



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:16 PM GMT

PDB ID : 4HRI
Title : Crystal structure of HetR in complex with a 21-bp palindromic DNA at the upstream of the hetP promoter from Anabaena
Authors : Hu, H.X.; Jiang, Y.L.; Zhao, M.X.; Chen, Y.; Zhang, C.C.; Zhou, C.Z.
Deposited on : 2012-10-28
Resolution : 2.95 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

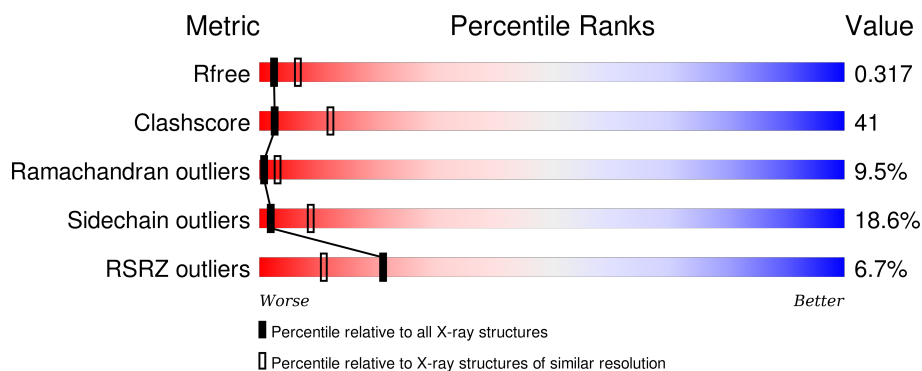
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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 ≥ 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.

Mol	Chain	Length	Quality of chain
1	A	307	<div> <div>9%</div> <div>36%</div> <div>37%</div> <div>14%</div> <div>•</div> <div>11%</div> </div>
1	B	307	<div> <div>4%</div> <div>35%</div> <div>36%</div> <div>18%</div> <div>•</div> <div>9%</div> </div>
2	C	21	<div> <div>24%</div> <div>67%</div> <div>10%</div> </div>
3	D	21	<div> <div>5%</div> <div>14%</div> <div>48%</div> <div>38%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5417 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 Heterocyst differentiation control protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	280	Total	C	N	O	S	0	0	0
			2296	1468	400	411	17			
1	A	272	Total	C	N	O	S	0	0	0
			2257	1442	393	405	17			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	MET	-	EXPRESSION TAG	UNP P27709
B	-6	GLY	-	EXPRESSION TAG	UNP P27709
B	-5	HIS	-	EXPRESSION TAG	UNP P27709
B	-4	HIS	-	EXPRESSION TAG	UNP P27709
B	-3	HIS	-	EXPRESSION TAG	UNP P27709
B	-2	HIS	-	EXPRESSION TAG	UNP P27709
B	-1	HIS	-	EXPRESSION TAG	UNP P27709
B	0	HIS	-	EXPRESSION TAG	UNP P27709
A	-7	MET	-	EXPRESSION TAG	UNP P27709
A	-6	GLY	-	EXPRESSION TAG	UNP P27709
A	-5	HIS	-	EXPRESSION TAG	UNP P27709
A	-4	HIS	-	EXPRESSION TAG	UNP P27709
A	-3	HIS	-	EXPRESSION TAG	UNP P27709
A	-2	HIS	-	EXPRESSION TAG	UNP P27709
A	-1	HIS	-	EXPRESSION TAG	UNP P27709
A	0	HIS	-	EXPRESSION TAG	UNP P27709

- Molecule 2 is a DNA chain called DNA (5'-D(P*GP*CP*GP*AP*GP*GP*GP*TP*C P*TP*AP*AP*CP*CP*CP*CP*TP*CP*AP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	21	Total	C	N	O	P	0	0	0
			425	199	79	126	21			

- Molecule 3 is a DNA chain called DNA (5'-D(P*AP*TP*GP*AP*GP*GP*GP*GP*TP*TP*AP*GP*AP*CP*CP*CP*CP*TP*CP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	21	Total	C	N	O	P	0	0	0
			430	202	81	126	21			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Ca	0	0
			1	1		
4	C	2	Total	Ca	0	0
			2	2		

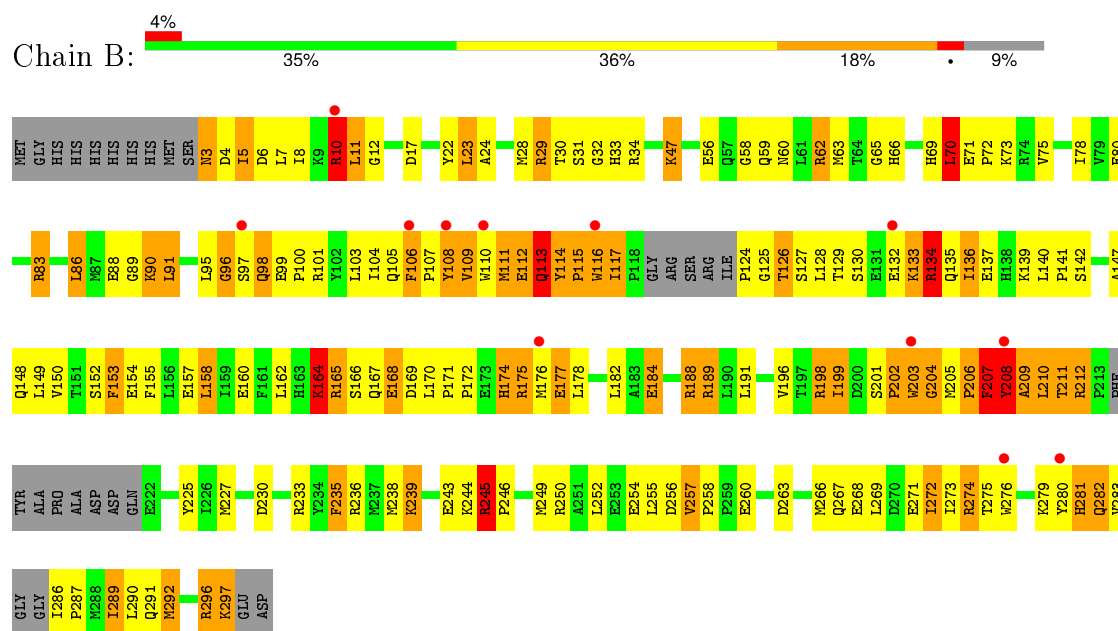
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	3	Total	O	0	0
			3	3		
5	A	2	Total	O	0	0
			2	2		
5	D	1	Total	O	0	0
			1	1		

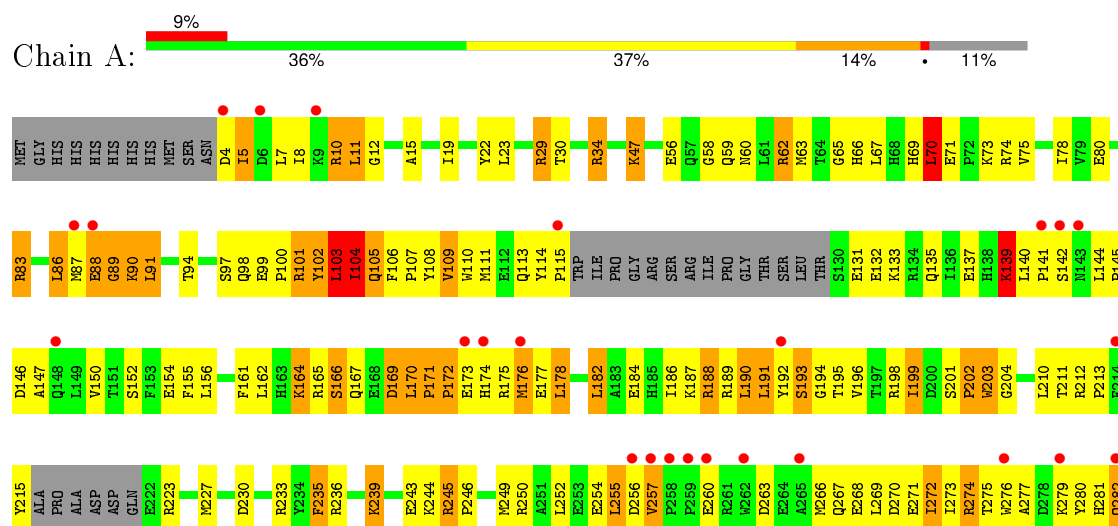
3 Residue-property plots

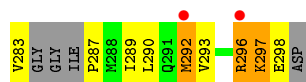
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

• Molecule 1: Heterocyst differentiation control protein

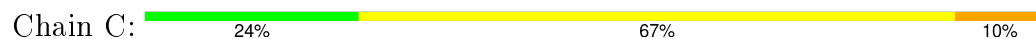


• Molecule 1: Heterocyst differentiation control protein

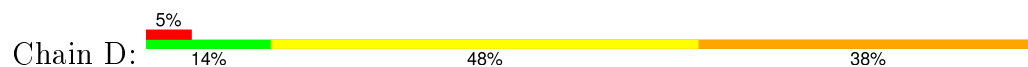




- Molecule 2: DNA (5'-D(P*GP*CP*GP*AP*GP*GP*GP*GP*TP*CP*TP*AP*AP*CP*CP*CP*CP*TP*CP*AP*T)-3')



- Molecule 3: DNA (5'-D(P*AP*TP*GP*AP*GP*GP*GP*GP*TP*TP*AP*GP*AP*CP*CP*CP*CP*TP*CP*GP*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	89.88 Å 89.88 Å 242.29 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.08 – 2.95 34.08 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.8 (34.08-2.95) 98.9 (34.08-2.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.95 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.231 , 0.307 0.248 , 0.317	Depositor DCC
R_{free} test set	1099 reflections (5.40%)	DCC
Wilson B-factor (Å ²)	89.9	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 101.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 21434 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5417	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.44	0/2311	1.01	19/3114 (0.6%)
1	B	0.44	0/2351	1.02	19/3174 (0.6%)
2	C	0.83	0/476	1.72	13/730 (1.8%)
3	D	0.87	0/482	1.94	25/741 (3.4%)
All	All	0.53	0/5620	1.21	76/7759 (1.0%)

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	5

There are no bond length outliers.

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	ARG	NE-CZ-NH1	-13.93	113.33	120.30
1	A	62	ARG	NE-CZ-NH2	13.70	127.15	120.30
1	B	34	ARG	NE-CZ-NH2	-12.93	113.83	120.30
1	A	34	ARG	NE-CZ-NH1	-12.79	113.91	120.30
1	A	29	ARG	NE-CZ-NH2	-12.29	114.15	120.30
1	A	245	ARG	NE-CZ-NH1	-12.16	114.22	120.30
1	A	10	ARG	NE-CZ-NH1	12.03	126.32	120.30
1	B	29	ARG	NE-CZ-NH1	-11.93	114.33	120.30
1	A	10	ARG	NE-CZ-NH2	-11.93	114.34	120.30
1	B	245	ARG	NE-CZ-NH2	-11.73	114.44	120.30
1	B	10	ARG	NE-CZ-NH1	-11.73	114.44	120.30
1	B	62	ARG	NE-CZ-NH2	-11.67	114.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	10	ARG	NE-CZ-NH2	11.63	126.12	120.30
1	A	245	ARG	NE-CZ-NH2	11.53	126.07	120.30
1	A	29	ARG	NE-CZ-NH1	11.21	125.91	120.30
1	B	245	ARG	NE-CZ-NH1	11.10	125.85	120.30
1	B	62	ARG	NE-CZ-NH1	11.03	125.82	120.30
1	B	34	ARG	NE-CZ-NH1	10.96	125.78	120.30
1	B	83	ARG	NE-CZ-NH2	10.86	125.73	120.30
1	A	83	ARG	NE-CZ-NH1	10.81	125.70	120.30
1	B	83	ARG	NE-CZ-NH1	-10.79	114.90	120.30
1	A	34	ARG	NE-CZ-NH2	10.76	125.68	120.30
1	A	83	ARG	NE-CZ-NH2	-10.75	114.92	120.30
1	B	29	ARG	NE-CZ-NH2	10.51	125.56	120.30
2	C	16	DC	O4'-C4'-C3'	-9.99	100.00	106.00
3	D	3	DG	O4'-C1'-N9	-9.56	101.31	108.00
3	D	14	DC	O4'-C4'-C3'	-9.53	100.28	106.00
3	D	11	DA	O4'-C1'-N9	-9.10	101.63	108.00
2	C	8	DG	O4'-C4'-C3'	-8.33	101.00	106.00
2	C	12	DA	O4'-C1'-N9	7.88	113.52	108.00
3	D	21	DC	O4'-C1'-N1	7.61	113.33	108.00
2	C	14	DC	O4'-C4'-C3'	-7.58	101.45	106.00
3	D	10	DT	C5-C4-O4	-7.52	119.64	124.90
2	C	5	DG	O4'-C1'-N9	7.48	113.24	108.00
2	C	15	DC	O4'-C4'-C3'	-7.32	101.57	104.50
3	D	13	DA	O4'-C4'-C3'	-7.31	101.58	104.50
2	C	21	DT	O4'-C4'-C3'	-7.25	101.60	104.50
3	D	10	DT	N3-C4-O4	7.15	124.19	119.90
3	D	20	DG	C3'-C2'-C1'	-7.14	93.93	102.50
3	D	16	DC	O4'-C4'-C3'	-7.08	101.67	104.50
3	D	20	DG	C4'-C3'-C2'	-7.08	96.72	103.10
3	D	16	DC	C4'-C3'-C2'	-6.80	96.98	103.10
3	D	13	DA	C4'-C3'-C2'	-6.68	97.09	103.10
2	C	12	DA	C3'-C2'-C1'	-6.68	94.49	102.50
1	A	62	ARG	CD-NE-CZ	6.62	132.86	123.60
3	D	9	DT	N3-C4-O4	6.58	123.85	119.90
3	D	4	DA	O4'-C1'-N9	6.37	112.46	108.00
2	C	5	DG	C1'-O4'-C4'	-6.36	103.74	110.10
3	D	16	DC	C1'-O4'-C4'	-6.35	103.75	110.10
3	D	13	DA	P-O5'-C5'	-6.34	110.75	120.90
1	B	70	LEU	CA-CB-CG	6.33	129.87	115.30
3	D	19	DC	O4'-C1'-N1	6.33	112.43	108.00
1	A	70	LEU	CA-CB-CG	6.17	129.48	115.30
1	B	10	ARG	CD-NE-CZ	6.16	132.22	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	14	DC	C4'-C3'-C2'	-6.11	97.60	103.10
1	A	245	ARG	CD-NE-CZ	5.99	131.99	123.60
1	A	10	ARG	CD-NE-CZ	5.99	131.98	123.60
1	B	62	ARG	CD-NE-CZ	5.96	131.94	123.60
3	D	19	DC	C3'-C2'-C1'	-5.93	95.39	102.50
1	B	34	ARG	CD-NE-CZ	5.83	131.76	123.60
1	B	245	ARG	CD-NE-CZ	5.78	131.69	123.60
2	C	19	DC	C3'-C2'-C1'	-5.75	95.60	102.50
3	D	9	DT	C5-C4-O4	-5.69	120.91	124.90
1	A	34	ARG	CD-NE-CZ	5.66	131.52	123.60
2	C	16	DC	C1'-O4'-C4'	-5.57	104.53	110.10
3	D	20	DG	O4'-C4'-C3'	-5.50	102.30	104.50
3	D	10	DT	O4'-C1'-N1	-5.42	104.20	108.00
1	B	83	ARG	CD-NE-CZ	5.41	131.17	123.60
1	A	29	ARG	CD-NE-CZ	5.36	131.11	123.60
2	C	5	DG	C4'-C3'-C2'	-5.36	98.28	103.10
3	D	18	DT	O4'-C1'-N1	5.31	111.72	108.00
3	D	3	DG	P-O5'-C5'	-5.29	112.44	120.90
2	C	12	DA	C4'-C3'-C2'	-5.25	98.38	103.10
1	A	83	ARG	CD-NE-CZ	5.21	130.89	123.60
3	D	7	DG	O4'-C4'-C3'	-5.14	102.44	104.50
1	B	29	ARG	CD-NE-CZ	5.09	130.72	123.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	108	TYR	Peptide
1	B	113	GLN	Peptide
1	B	206	PRO	Peptide
1	B	207	PHE	Peptide
1	B	96	GLY	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	2257	0	2236	188	0
1	B	2296	0	2286	269	0
2	C	425	0	224	15	0
3	D	430	0	230	19	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
5	A	2	0	0	1	0
5	B	3	0	0	2	0
5	D	1	0	0	1	0
All	All	5417	0	4976	427	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 (427) 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:108:TYR:HA	1:B:111:MET:HB3	1.29	1.14
1:B:175:ARG:HG2	1:B:175:ARG:HH11	1.10	1.10
1:B:211:THR:HG23	1:B:212:ARG:HD2	1.14	1.09
1:A:62:ARG:NH1	3:D:3:DG:N7	2.02	1.05
1:B:245:ARG:HG3	1:B:246:PRO:HD2	1.36	1.04
1:B:10:ARG:NH2	1:A:86:LEU:O	1.99	0.95
1:B:135:GLN:NE2	5:B:302:HOH:O	2.00	0.93
1:B:150:VAL:HG22	1:B:207:PHE:HD2	1.29	0.93
1:A:101:ARG:O	1:A:162:LEU:HD23	1.70	0.91
1:B:3:ASN:O	1:B:5:ILE:N	2.02	0.91
1:A:194:GLY:O	1:A:196:VAL:N	2.02	0.91
1:B:95:LEU:O	1:B:97:SER:N	2.06	0.89
1:B:198:ARG:CZ	1:B:206:PRO:HG3	2.03	0.88
1:A:194:GLY:O	1:A:196:VAL:HG23	1.74	0.88
1:B:111:MET:HG2	1:B:207:PHE:CE1	2.07	0.88
1:A:105:GLN:HE22	1:A:210:LEU:HD21	1.40	0.87
1:A:184:GLU:O	1:A:188:ARG:HG2	1.76	0.86
1:B:3:ASN:N	1:B:6:ASP:OD2	2.09	0.86
1:B:198:ARG:NH2	1:B:206:PRO:HG3	1.89	0.85
1:A:282:GLN:HG3	1:A:283:VAL:H	1.39	0.85
1:A:245:ARG:HG3	1:A:246:PRO:HD2	1.57	0.85
1:A:104:ILE:HD13	1:A:106:PHE:HD2	1.41	0.85
1:A:98:GLN:HB3	1:A:99:GLU:HB3	1.60	0.84
1:B:66:HIS:HB3	1:A:188:ARG:HG3	1.60	0.83
1:B:257:VAL:HG13	1:A:287:PRO:HD3	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:ARG:HG2	1:B:175:ARG:NH1	1.78	0.82
1:A:243:GLU:OE2	1:A:245:ARG:NH1	2.13	0.82
1:B:47:LYS:HD3	1:B:78:ILE:HG12	1.63	0.81
1:B:86:LEU:O	1:A:10:ARG:NH2	2.13	0.81
1:B:175:ARG:CG	1:B:175:ARG:HH11	1.93	0.81
1:A:164:LYS:HE3	1:A:164:LYS:HA	1.63	0.80
1:B:136:ILE:HG12	1:B:139:LYS:HE2	1.63	0.80
2:C:11:DT:O4	3:D:11:DA:N6	2.14	0.80
1:B:108:TYR:HB2	5:B:301:HOH:O	1.82	0.80
1:B:108:TYR:CA	1:B:111:MET:HB3	2.11	0.80
1:A:203:TRP:O	1:A:203:TRP:CD1	2.35	0.80
1:B:167:GLN:HG2	1:B:170:LEU:HD12	1.62	0.79
1:B:203:TRP:CG	1:B:204:GLY:N	2.51	0.79
1:B:108:TYR:HA	1:B:111:MET:H	1.48	0.78
1:B:126:THR:O	1:B:134:ARG:NH1	2.13	0.78
1:B:33:HIS:NE2	1:B:99:GLU:O	2.17	0.78
1:A:98:GLN:N	1:A:98:GLN:OE1	2.17	0.77
1:A:203:TRP:O	1:A:203:TRP:HD1	1.66	0.76
1:B:31:SER:CB	1:B:99:GLU:HB3	2.14	0.76
1:B:175:ARG:HG3	1:B:176:MET:H	1.51	0.75
1:B:111:MET:HG2	1:B:207:PHE:CZ	2.22	0.74
1:B:172:PRO:HA	1:B:175:ARG:HB2	1.68	0.74
1:B:107:PRO:HB2	1:B:108:TYR:CZ	2.21	0.74
1:B:114:TYR:HB3	1:B:115:PRO:HD2	1.68	0.74
1:A:263:ASP:O	1:A:267:GLN:HB2	1.88	0.74
1:B:107:PRO:HB2	1:B:108:TYR:CE1	2.22	0.73
1:B:206:PRO:O	1:B:207:PHE:HB2	1.85	0.73
1:A:47:LYS:HD3	1:A:78:ILE:HG12	1.69	0.73
1:B:112:GLU:OE1	1:B:147:ALA:HB2	1.90	0.71
2:C:17:DC:O2	3:D:5:DG:N2	2.19	0.71
1:B:89:GLY:O	1:B:91:LEU:N	2.23	0.71
1:B:31:SER:HB3	1:B:99:GLU:HB3	1.72	0.71
1:B:113:GLN:O	1:B:114:TYR:CG	2.43	0.71
1:A:89:GLY:O	1:A:91:LEU:N	2.24	0.71
1:B:65:GLY:HA2	1:B:70:LEU:HD13	1.73	0.71
1:B:129:THR:HB	1:B:133:LYS:NZ	2.06	0.71
1:B:170:LEU:O	1:B:175:ARG:NE	2.21	0.70
1:A:8:ILE:O	1:A:12:GLY:N	2.20	0.70
1:B:135:GLN:HA	1:B:135:GLN:OE1	1.89	0.70
3:D:16:DC:H2'	3:D:17:DC:H6	1.55	0.70
1:B:165:ARG:O	1:B:168:GLU:HG2	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:ASP:O	1:B:267:GLN:HB2	1.92	0.69
1:B:107:PRO:HB3	1:B:162:LEU:HG	1.75	0.69
1:B:108:TYR:HE2	1:B:158:LEU:HG	1.56	0.69
1:B:125:GLY:HA3	1:B:134:ARG:HD3	1.75	0.69
1:A:102:TYR:O	1:A:103:LEU:HB3	1.93	0.69
1:B:116:TRP:HA	1:B:147:ALA:HA	1.75	0.69
1:B:150:VAL:HG22	1:B:207:PHE:CD2	2.21	0.68
1:B:188:ARG:HG3	1:A:63:MET:HE3	1.75	0.68
3:D:10:DT:H2''	3:D:11:DA:C8	2.28	0.68
1:B:175:ARG:HG3	1:B:176:MET:HG2	1.76	0.67
1:B:254:GLU:HG2	1:A:289:ILE:HD13	1.77	0.67
1:B:281:HIS:O	1:B:282:GLN:HG2	1.94	0.67
1:A:99:GLU:OE1	1:A:99:GLU:N	2.28	0.67
1:B:167:GLN:OE1	1:B:176:MET:HA	1.95	0.67
1:B:8:ILE:O	1:B:12:GLY:N	2.21	0.67
1:A:102:TYR:O	1:A:103:LEU:CB	2.43	0.67
1:B:154:GLU:HG2	1:B:157:GLU:OE1	1.94	0.67
1:A:133:LYS:HA	1:A:135:GLN:H	1.60	0.67
1:A:145:PRO:HG3	1:A:213:PRO:HG3	1.75	0.66
1:B:292:MET:SD	1:A:290:LEU:HD11	2.35	0.66
1:B:133:LYS:O	1:B:135:GLN:N	2.28	0.66
1:B:101:ARG:O	1:B:105:GLN:HB2	1.96	0.66
1:B:99:GLU:HB2	1:B:100:PRO:HD3	1.78	0.66
1:B:167:GLN:O	1:B:169:ASP:N	2.30	0.65
1:B:133:LYS:HB2	1:B:133:LYS:NZ	2.12	0.65
1:A:245:ARG:CG	1:A:246:PRO:HD2	2.24	0.65
1:A:74:ARG:HH21	2:C:12:DA:H3'	1.62	0.64
1:B:235:PHE:HE2	1:A:227:MET:HE2	1.63	0.64
1:B:133:LYS:C	1:B:135:GLN:H	2.00	0.64
1:B:108:TYR:O	1:B:208:TYR:OH	2.15	0.64
1:A:139:LYS:O	1:A:141:PRO:HD3	1.98	0.64
1:B:137:GLU:HA	1:B:140:LEU:HD12	1.79	0.64
1:B:126:THR:OG1	1:B:127:SER:N	2.30	0.64
1:B:108:TYR:HA	1:B:111:MET:CB	2.16	0.63
1:A:155:PHE:CE2	1:A:187:LYS:HG3	2.33	0.63
1:B:109:VAL:O	1:B:113:GLN:NE2	2.30	0.63
1:B:62:ARG:NH1	2:C:3:DG:N7	2.46	0.63
1:B:111:MET:HE2	1:B:207:PHE:CD1	2.33	0.63
1:A:139:LYS:H	1:A:139:LYS:NZ	1.97	0.63
1:B:245:ARG:HG3	1:B:246:PRO:CD	2.21	0.63
1:A:150:VAL:HB	1:A:154:GLU:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ARG:HD2	1:A:87:MET:HG3	1.79	0.63
1:B:290:LEU:HD11	1:A:292:MET:SD	2.39	0.63
1:B:243:GLU:OE2	1:B:245:ARG:NH1	2.31	0.63
1:B:130:SER:H	1:B:133:LYS:HZ2	1.46	0.63
1:B:164:LYS:HE3	1:B:164:LYS:N	2.13	0.62
1:B:129:THR:HB	1:B:133:LYS:HZ3	1.65	0.61
1:A:172:PRO:HA	1:A:175:ARG:HG2	1.81	0.61
1:B:130:SER:H	1:B:133:LYS:NZ	1.98	0.61
1:A:65:GLY:HA2	1:A:70:LEU:HD13	1.82	0.61
1:B:290:LEU:O	1:A:252:LEU:HA	2.01	0.61
1:B:111:MET:HE1	1:B:207:PHE:CG	2.36	0.60
1:A:105:GLN:NE2	1:A:210:LEU:HD21	2.14	0.60
1:B:100:PRO:HB2	1:B:105:GLN:OE1	2.00	0.60
1:B:108:TYR:CA	1:B:111:MET:H	2.14	0.60
1:B:175:ARG:HG3	1:B:176:MET:N	2.14	0.60
1:A:80:GLU:OE2	1:A:83:ARG:NH2	2.35	0.60
1:B:111:MET:HE1	1:B:207:PHE:CD2	2.36	0.60
1:B:177:GLU:N	1:B:177:GLU:OE2	2.34	0.60
1:B:104:ILE:C	1:B:107:PRO:HD3	2.22	0.60
1:B:208:TYR:O	1:B:209:ALA:CB	2.49	0.60
1:B:209:ALA:O	1:B:210:LEU:O	2.20	0.60
1:A:194:GLY:C	1:A:196:VAL:H	2.03	0.59
1:A:155:PHE:HE2	1:A:187:LYS:HG3	1.67	0.59
1:A:267:GLN:O	1:A:270:ASP:OD2	2.21	0.59
1:B:108:TYR:N	1:B:108:TYR:CD2	2.68	0.59
1:A:279:LYS:HD3	1:A:280:TYR:CE2	2.37	0.59
1:B:286:ILE:HB	1:A:257:VAL:O	2.01	0.59
1:B:3:ASN:N	1:B:3:ASN:HD22	2.01	0.59
1:A:109:VAL:O	1:A:113:GLN:CD	2.41	0.59
3:D:14:DC:OP2	5:D:201:HOH:O	2.16	0.59
1:B:256:ASP:HB2	1:A:281:HIS:CE1	2.38	0.59
1:A:74:ARG:NH2	2:C:12:DA:H3'	2.19	0.58
1:B:266:MET:HG3	1:A:249:MET:SD	2.42	0.58
1:A:281:HIS:O	1:A:282:GLN:CB	2.52	0.58
1:B:184:GLU:HB3	1:A:66:HIS:CD2	2.38	0.58
1:B:236:ARG:HG3	1:A:22:TYR:OH	2.04	0.58
1:B:150:VAL:CG2	1:B:207:PHE:HD2	2.10	0.58
3:D:16:DC:H2'	3:D:17:DC:C6	2.36	0.58
1:B:188:ARG:HG3	1:A:63:MET:CE	2.33	0.58
1:B:279:LYS:HD3	1:B:280:TYR:CE2	2.38	0.58
1:A:102:TYR:CE1	1:A:215:TYR:O	2.56	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ASN:ND2	1:B:63:MET:HB2	2.19	0.58
1:B:133:LYS:C	1:B:135:GLN:N	2.58	0.57
1:B:107:PRO:C	1:B:108:TYR:CG	2.74	0.57
1:B:111:MET:HE2	1:B:207:PHE:CE1	2.39	0.57
1:A:60:ASN:ND2	1:A:63:MET:HB2	2.20	0.57
1:A:139:LYS:HZ3	1:A:139:LYS:H	1.51	0.57
1:A:145:PRO:HD2	1:A:210:LEU:O	2.05	0.57
1:B:111:MET:CG	1:B:207:PHE:CZ	2.86	0.57
1:A:189:ARG:O	1:A:193:SER:O	2.22	0.57
3:D:17:DC:H2''	3:D:18:DT:H5'	1.86	0.57
1:B:133:LYS:HB2	1:B:133:LYS:HZ2	1.67	0.57
1:B:157:GLU:O	1:B:160:GLU:HG2	2.05	0.56
1:B:31:SER:HB2	1:B:99:GLU:C	2.25	0.56
1:B:235:PHE:CE2	1:A:227:MET:HE2	2.40	0.56
1:A:34:ARG:HG3	1:A:101:ARG:HH22	1.70	0.56
1:B:175:ARG:O	1:B:177:GLU:OE2	2.24	0.56
1:B:124:PRO:HA	1:B:149:LEU:HB2	1.88	0.56
1:A:70:LEU:HD22	1:A:75:VAL:HG22	1.88	0.56
1:B:281:HIS:CG	1:B:282:GLN:H	2.24	0.56
1:A:47:LYS:HD2	1:A:78:ILE:HG23	1.88	0.56
1:B:98:GLN:OE1	1:B:225:TYR:HE2	1.89	0.56
1:A:198:ARG:HD2	1:A:199:ILE:H	1.71	0.56
1:A:282:GLN:HG3	1:A:283:VAL:N	2.18	0.55
1:B:110:TRP:HE1	1:B:165:ARG:HH11	1.54	0.55
1:A:202:PRO:HD2	1:A:203:TRP:H	1.71	0.55
1:A:73:LYS:NZ	3:D:6:DG:N7	2.54	0.55
1:B:198:ARG:HH11	1:B:198:ARG:HA	1.71	0.55
1:B:274:ARG:NH1	1:B:274:ARG:HB2	2.22	0.55
1:B:89:GLY:O	1:B:90:LYS:C	2.46	0.55
1:B:136:ILE:CG1	1:B:139:LYS:HE2	2.36	0.54
1:A:202:PRO:HG2	1:A:204:GLY:O	2.06	0.54
1:B:189:ARG:HH11	1:A:67:LEU:HD22	1.71	0.54
1:A:71:GLU:O	1:A:75:VAL:HG23	2.07	0.54
1:B:112:GLU:O	1:B:113:GLN:HB2	2.06	0.54
2:C:7:DG:H2'	2:C:8:DG:O4'	2.07	0.54
1:A:105:GLN:OE1	1:A:105:GLN:O	2.25	0.54
1:A:281:HIS:CG	1:A:282:GLN:H	2.25	0.54
1:B:110:TRP:HE1	1:B:165:ARG:NH1	2.05	0.54
1:B:113:GLN:O	1:B:114:TYR:CB	2.55	0.54
1:B:107:PRO:HB2	1:B:108:TYR:CE2	2.42	0.54
1:B:289:ILE:HG13	1:A:297:LYS:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:ARG:NH1	1:B:206:PRO:HG3	2.22	0.54
3:D:4:DA:H2''	3:D:5:DG:H5''	1.89	0.54
1:B:257:VAL:HG13	1:A:287:PRO:CD	2.36	0.54
1:B:114:TYR:CB	1:B:115:PRO:HD2	2.31	0.53
1:B:132:GLU:O	1:B:135:GLN:HG2	2.09	0.53
1:B:256:ASP:HB3	1:B:257:VAL:HG23	1.90	0.53
3:D:17:DC:H5''	3:D:17:DC:C6	2.44	0.53
1:B:106:PHE:O	1:B:110:TRP:HD1	1.92	0.53
1:B:111:MET:CE	1:B:207:PHE:CD1	2.92	0.53
1:B:167:GLN:HB3	1:B:175:ARG:HD2	1.90	0.53
3:D:1:DA:H1'	3:D:2:DT:H5''	1.91	0.53
1:B:32:GLY:CA	1:B:189:ARG:HH21	2.21	0.52
2:C:3:DG:H2'	2:C:4:DA:H8	1.74	0.52
1:A:191:LEU:O	1:A:193:SER:O	2.27	0.52
2:C:3:DG:H2''	2:C:4:DA:C5'	2.40	0.52
1:B:107:PRO:HB2	1:B:108:TYR:CD1	2.45	0.52
1:A:99:GLU:O	1:A:99:GLU:HG2	2.08	0.52
2:C:2:DC:H2'	2:C:3:DG:C8	2.44	0.52
1:A:245:ARG:HG3	1:A:246:PRO:CD	2.33	0.52
1:B:227:MET:HE2	1:A:235:PHE:HE2	1.74	0.52
1:B:17:ASP:OD2	1:A:94:THR:HB	2.10	0.52
1:B:292:MET:CE	1:A:290:LEU:HD11	2.40	0.52
1:B:202:PRO:O	1:B:203:TRP:HB2	2.09	0.52
1:B:112:GLU:O	1:B:113:GLN:CB	2.57	0.52
1:B:188:ARG:HH11	1:B:191:LEU:HD12	1.75	0.52
1:B:56:GLU:CD	1:A:29:ARG:HH22	2.13	0.52
1:B:139:LYS:HG3	1:B:139:LYS:O	2.10	0.51
1:B:8:ILE:N	1:B:8:ILE:HD12	2.24	0.51
1:A:255:LEU:N	1:A:255:LEU:HD23	2.25	0.51
1:A:62:ARG:HE	3:D:2:DT:H2'	1.75	0.51
1:A:8:ILE:HD12	1:A:8:ILE:N	2.25	0.51
1:B:227:MET:HE1	1:A:239:LYS:CG	2.40	0.51
1:B:7:LEU:HD13	1:A:86:LEU:HD21	1.93	0.51
1:A:7:LEU:O	1:A:11:LEU:HB2	2.10	0.51
1:A:5:ILE:HA	1:A:8:ILE:HD13	1.93	0.51
1:B:207:PHE:HD1	1:B:208:TYR:CB	2.24	0.51
1:B:164:LYS:O	1:B:166:SER:N	2.44	0.51
1:A:107:PRO:HG2	1:A:162:LEU:HD13	1.92	0.51
1:A:268:GLU:O	1:A:272:ILE:HG23	2.11	0.51
1:B:211:THR:OG1	1:B:211:THR:O	2.26	0.50
1:B:201:SER:C	1:B:203:TRP:H	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:TRP:CD2	1:B:204:GLY:N	2.70	0.50
1:A:169:ASP:O	1:A:170:LEU:C	2.49	0.50
1:B:297:LYS:HG2	1:A:289:ILE:HG13	1.94	0.50
1:A:172:PRO:O	1:A:173:GLU:HB3	2.11	0.50
1:B:167:GLN:C	1:B:169:ASP:N	2.65	0.50
1:B:3:ASN:N	1:B:6:ASP:CG	2.65	0.50
1:A:172:PRO:C	1:A:174:HIS:H	2.15	0.50
1:B:32:GLY:HA2	1:B:189:ARG:HH21	1.76	0.50
1:B:108:TYR:CE2	1:B:158:LEU:HG	2.42	0.50
1:B:133:LYS:CB	1:B:133:LYS:NZ	2.74	0.50
1:B:7:LEU:O	1:B:11:LEU:HB2	2.12	0.50
1:A:104:ILE:HG23	1:A:104:ILE:O	2.12	0.50
1:B:70:LEU:HD22	1:B:75:VAL:HG22	1.92	0.50
1:A:103:LEU:C	1:A:105:GLN:H	2.15	0.50
1:B:80:GLU:OE2	1:B:83:ARG:NH2	2.45	0.50
1:A:58:GLY:O	1:A:59:GLN:HB2	2.11	0.50
1:B:268:GLU:O	1:B:272:ILE:HG23	2.12	0.49
1:B:104:ILE:O	1:B:107:PRO:CD	2.59	0.49
1:B:5:ILE:HA	1:B:8:ILE:HD13	1.93	0.49
1:B:108:TYR:HA	1:B:111:MET:N	2.21	0.49
1:B:111:MET:O	1:B:111:MET:SD	2.70	0.49
1:B:252:LEU:HA	1:A:290:LEU:O	2.13	0.49
1:A:109:VAL:O	1:A:113:GLN:OE1	2.31	0.49
1:B:289:ILE:HG23	1:A:252:LEU:HD11	1.94	0.49
1:B:104:ILE:C	1:B:107:PRO:CD	2.81	0.49
3:D:17:DC:H5"	3:D:17:DC:H6	1.78	0.48
1:A:282:GLN:CG	1:A:283:VAL:H	2.17	0.48
1:B:289:ILE:CG1	1:A:297:LYS:HG2	2.43	0.48
1:B:56:GLU:OE1	1:A:29:ARG:NH2	2.46	0.48
1:A:274:ARG:NH1	1:A:274:ARG:HB2	2.28	0.48
1:A:104:ILE:HD13	1:A:106:PHE:CD2	2.33	0.48
1:B:230:ASP:OD1	1:B:233:ARG:NH2	2.46	0.48
1:B:255:LEU:HD23	1:B:255:LEU:N	2.29	0.48
1:A:145:PRO:O	1:A:147:ALA:N	2.47	0.48
1:B:31:SER:O	1:B:100:PRO:HA	2.13	0.48
1:B:66:HIS:CB	1:A:188:ARG:HG3	2.38	0.48
1:A:88:GLU:O	1:A:90:LYS:N	2.47	0.48
1:B:257:VAL:CG1	1:A:287:PRO:HD3	2.40	0.48
1:B:281:HIS:O	1:B:282:GLN:CG	2.62	0.48
1:B:289:ILE:HG23	1:A:252:LEU:CD1	2.44	0.48
1:A:131:GLU:O	1:A:132:GLU:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:GLY:O	1:A:69:HIS:N	2.47	0.47
1:B:107:PRO:HG2	1:B:108:TYR:CD1	2.49	0.47
1:B:108:TYR:HD2	1:B:111:MET:CB	2.27	0.47
1:B:167:GLN:OE1	1:B:176:MET:CA	2.62	0.47
3:D:18:DT:H2''	3:D:19:DC:C6	2.49	0.47
1:B:58:GLY:O	1:B:59:GLN:HB2	2.14	0.47
2:C:11:DT:C4	3:D:11:DA:N1	2.81	0.47
1:B:116:TRP:CD2	1:B:116:TRP:N	2.83	0.47
1:B:29:ARG:HH22	1:A:56:GLU:CD	2.18	0.47
1:B:182:LEU:HD13	1:A:69:HIS:CE1	2.50	0.47
1:B:111:MET:CE	1:B:207:PHE:CE1	2.97	0.47
1:A:252:LEU:HD12	1:A:252:LEU:C	2.35	0.47
1:A:177:GLU:N	1:A:177:GLU:OE1	2.47	0.47
1:A:175:ARG:O	1:A:176:MET:HB3	2.13	0.47
1:B:56:GLU:CD	1:A:29:ARG:NH2	2.68	0.47
1:A:178:LEU:HD12	1:A:178:LEU:HA	1.69	0.47
1:B:108:TYR:CB	1:B:111:MET:HB3	2.45	0.47
1:B:116:TRP:N	1:B:148:GLN:HG2	2.30	0.47
1:B:167:GLN:C	1:B:169:ASP:H	2.17	0.47
1:B:207:PHE:HD1	1:B:208:TYR:HB2	1.80	0.46
1:B:139:LYS:O	1:B:140:LEU:HG	2.16	0.46
1:B:22:TYR:OH	1:A:236:ARG:HG3	2.16	0.46
1:B:104:ILE:O	1:B:107:PRO:HD2	2.15	0.46
1:B:141:PRO:O	1:B:142:SER:OG	2.21	0.46
1:B:24:ALA:O	1:B:28:MET:HB2	2.16	0.46
1:B:108:TYR:CD2	1:B:111:MET:HB2	2.51	0.46
1:A:100:PRO:O	1:A:101:ARG:C	2.54	0.46
1:B:31:SER:HB2	1:B:99:GLU:HB3	1.94	0.46
1:A:8:ILE:H	1:A:8:ILE:HD12	1.80	0.46
1:B:189:ARG:HD2	1:B:189:ARG:HA	1.54	0.46
1:B:274:ARG:HH11	1:B:274:ARG:HB2	1.81	0.46
1:A:274:ARG:O	1:A:277:ALA:N	2.48	0.46
1:B:152:SER:HB2	1:B:203:TRP:CZ2	2.51	0.46
1:A:198:ARG:HA	1:A:198:ARG:HD2	1.69	0.46
1:B:297:LYS:HG2	1:A:289:ILE:CG1	2.46	0.46
1:B:110:TRP:NE1	1:B:165:ARG:NH1	2.64	0.45
2:C:3:DG:H2'	2:C:4:DA:C8	2.50	0.45
1:A:296:ARG:HB3	1:A:297:LYS:H	1.63	0.45
1:B:171:PRO:HB2	1:B:174:HIS:CE1	2.50	0.45
1:B:207:PHE:HD1	1:B:208:TYR:CG	2.34	0.45
1:A:10:ARG:O	1:A:10:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:LYS:HA	1:A:135:GLN:N	2.29	0.45
1:B:114:TYR:HB3	1:B:115:PRO:CD	2.43	0.45
2:C:3:DG:H2''	2:C:4:DA:O5'	2.15	0.45
1:B:141:PRO:O	1:B:142:SER:CB	2.64	0.45
1:B:132:GLU:CD	1:B:132:GLU:H	2.18	0.45
1:B:137:GLU:HA	1:B:140:LEU:CD1	2.46	0.45
1:B:8:ILE:HD12	1:B:8:ILE:H	1.81	0.45
1:A:230:ASP:OD1	1:A:233:ARG:NH2	2.50	0.45
1:B:208:TYR:HD1	1:B:208:TYR:HA	1.59	0.45
1:A:63:MET:HE2	1:A:67:LEU:HG	1.99	0.45
1:B:177:GLU:N	1:B:177:GLU:CD	2.70	0.45
1:A:34:ARG:HD3	1:A:182:LEU:HD21	1.98	0.45
1:B:108:TYR:CD2	1:B:111:MET:CB	3.00	0.45
1:B:208:TYR:O	1:B:209:ALA:HB2	2.17	0.45
1:B:69:HIS:CE1	1:A:182:LEU:HD23	2.52	0.44
1:B:65:GLY:O	1:B:69:HIS:N	2.50	0.44
1:A:105:GLN:C	1:A:105:GLN:OE1	2.56	0.44
3:D:10:DT:H2''	3:D:11:DA:H8	1.77	0.44
1:A:269:LEU:HD11	1:A:292:MET:HE3	1.99	0.44
1:B:116:TRP:CE3	1:B:116:TRP:N	2.85	0.44
1:B:238:MET:CE	1:A:227:MET:HA	2.46	0.44
1:A:191:LEU:HA	1:A:191:LEU:HD12	1.66	0.44
1:B:249:MET:SD	1:A:266:MET:HG3	2.57	0.44
1:A:276:TRP:O	1:A:279:LYS:HB3	2.17	0.44
1:A:198:ARG:HD2	1:A:199:ILE:N	2.30	0.44
1:B:203:TRP:O	1:B:204:GLY:C	2.55	0.44
1:A:269:LEU:HD11	1:A:292:MET:CE	2.47	0.44
1:A:106:PHE:O	1:A:110:TRP:HD1	2.00	0.44
1:B:66:HIS:CD2	1:A:184:GLU:HG2	2.52	0.44
1:B:286:ILE:HA	1:B:287:PRO:HD3	1.76	0.44
1:A:114:TYR:CD1	1:A:115:PRO:HD2	2.52	0.44
1:B:99:GLU:OE1	1:B:99:GLU:N	2.50	0.44
2:C:11:DT:O4	3:D:11:DA:C6	2.71	0.44
1:B:276:TRP:O	1:B:279:LYS:HB3	2.17	0.44
1:B:196:VAL:HA	1:B:208:TYR:H	1.83	0.44
1:A:99:GLU:CG	1:A:99:GLU:O	2.65	0.44
1:B:269:LEU:HD11	1:B:292:MET:CE	2.48	0.43
1:B:296:ARG:HB3	1:B:297:LYS:H	1.64	0.43
1:A:139:LYS:HG2	1:A:140:LEU:N	2.34	0.43
1:B:116:TRP:HA	1:B:147:ALA:CA	2.48	0.43
1:B:99:GLU:HB2	1:B:100:PRO:CD	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:ARG:NH1	1:B:191:LEU:HD12	2.33	0.43
1:B:154:GLU:HA	1:B:157:GLU:HB3	2.00	0.43
1:B:71:GLU:O	1:B:75:VAL:HG23	2.19	0.43
1:A:196:VAL:HG22	5:A:301:HOH:O	2.18	0.43
1:A:186:ILE:O	1:A:190:LEU:HD22	2.19	0.43
1:A:106:PHE:N	1:A:107:PRO:CD	2.82	0.43
1:B:112:GLU:H	1:B:112:GLU:HG2	1.54	0.43
1:B:209:ALA:O	1:B:210:LEU:C	2.57	0.43
1:A:100:PRO:HG2	1:A:166:SER:OG	2.19	0.43
1:A:137:GLU:O	1:A:137:GLU:HG2	2.19	0.43
1:B:137:GLU:O	1:B:137:GLU:HG2	2.18	0.42
1:B:71:GLU:HA	1:B:72:PRO:HD3	1.91	0.42
1:B:227:MET:HE2	1:A:235:PHE:CE2	2.52	0.42
1:A:161:PHE:C	1:A:161:PHE:CD2	2.92	0.42
1:A:212:ARG:HA	1:A:213:PRO:HD3	1.62	0.42
1:A:80:GLU:OE1	1:A:80:GLU:HA	2.19	0.42
1:B:80:GLU:HA	1:B:80:GLU:OE1	2.19	0.42
1:A:70:LEU:N	1:A:70:LEU:HD12	2.34	0.42
2:C:9:DT:H2''	2:C:10:DC:C6	2.54	0.42
1:B:107:PRO:O	1:B:108:TYR:CB	2.67	0.42
1:B:23:LEU:HD23	1:B:23:LEU:HA	1.68	0.42
1:A:297:LYS:O	1:A:298:GLU:HB3	2.19	0.42
1:B:3:ASN:O	1:B:6:ASP:OD2	2.38	0.42
1:A:202:PRO:O	1:A:203:TRP:HB3	2.20	0.42
1:A:165:ARG:C	1:A:167:GLN:N	2.72	0.42
1:A:223:ARG:HG2	1:A:223:ARG:H	1.66	0.42
1:B:47:LYS:HD2	1:B:78:ILE:HG23	2.01	0.42
1:A:192:TYR:O	1:A:193:SER:HB3	2.19	0.42
1:A:274:ARG:HA	1:A:274:ARG:HD3	1.93	0.42
1:B:207:PHE:CD1	1:B:208:TYR:CG	3.08	0.42
3:D:1:DA:P	3:D:1:DA:C8	3.12	0.42
1:A:106:PHE:O	1:A:110:TRP:CD1	2.72	0.42
1:B:257:VAL:HG22	1:A:287:PRO:N	2.35	0.42
1:B:239:LYS:HE2	1:A:4:ASP:OD1	2.20	0.42
1:B:198:ARG:HA	1:B:198:ARG:HD3	1.47	0.41
1:B:86:LEU:HD12	1:B:86:LEU:HA	1.92	0.41
2:C:12:DA:H2'	2:C:12:DA:O5'	2.20	0.41
1:A:201:SER:HA	1:A:202:PRO:HD3	1.63	0.41
1:B:99:GLU:CB	1:B:100:PRO:HD3	2.48	0.41
1:B:281:HIS:CE1	1:A:256:ASP:HB2	2.56	0.41
1:B:257:VAL:HB	1:A:283:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:LEU:HD11	1:B:292:MET:HE3	2.02	0.41
1:A:245:ARG:CD	1:A:246:PRO:HD2	2.49	0.41
1:B:289:ILE:HD13	1:A:254:GLU:HG2	2.02	0.41
1:B:177:GLU:H	1:B:177:GLU:CD	2.24	0.41
1:B:153:PHE:HD2	1:B:153:PHE:O	2.04	0.41
1:B:252:LEU:CD1	1:A:289:ILE:HG23	2.51	0.41
1:A:171:PRO:O	1:A:172:PRO:O	2.38	0.41
1:B:153:PHE:C	1:B:153:PHE:CD2	2.94	0.41
1:B:69:HIS:ND1	1:A:34:ARG:HD2	2.36	0.41
1:A:15:ALA:O	1:A:19:ILE:HG13	2.21	0.41
1:B:135:GLN:O	1:B:136:ILE:HB	2.20	0.41
1:A:210:LEU:HA	1:A:210:LEU:HD12	1.87	0.41
1:B:252:LEU:C	1:B:252:LEU:HD12	2.41	0.41
1:A:172:PRO:O	1:A:173:GLU:CB	2.69	0.41
1:B:199:ILE:HB	1:B:205:MET:O	2.20	0.41
1:B:106:PHE:N	1:B:107:PRO:CD	2.84	0.40
1:B:155:PHE:CD2	1:B:206:PRO:HG2	2.56	0.40
1:A:202:PRO:CD	1:A:203:TRP:H	2.32	0.40
1:B:291:GLN:HB2	1:A:293:VAL:HG12	2.02	0.40
1:B:154:GLU:O	1:B:158:LEU:HB2	2.20	0.40
1:B:115:PRO:HB3	1:B:148:GLN:O	2.22	0.40
1:A:165:ARG:O	1:A:167:GLN:N	2.54	0.40
1:B:5:ILE:O	1:B:8:ILE:N	2.53	0.40
1:B:66:HIS:NE2	1:A:184:GLU:HG2	2.37	0.40
1:B:178:LEU:HA	1:B:182:LEU:HD23	2.03	0.40
1:B:256:ASP:HB3	1:A:282:GLN:O	2.22	0.40
1:B:104:ILE:HA	1:B:107:PRO:HG3	2.02	0.40
1:B:108:TYR:N	1:B:110:TRP:H	2.20	0.40
1:B:111:MET:SD	1:B:207:PHE:CZ	3.15	0.40
1:A:164:LYS:CE	1:A:164:LYS:HA	2.32	0.40
1:A:203:TRP:C	1:A:203:TRP:CD1	2.95	0.40
1:A:139:LYS:N	1:A:139:LYS:HD3	2.37	0.40
1:A:175:ARG:HA	1:A:177:GLU:OE2	2.22	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	264/307 (86%)	212 (80%)	30 (11%)	22 (8%)	1	4
1	B	272/307 (89%)	212 (78%)	31 (11%)	29 (11%)	0	2
All	All	536/614 (87%)	424 (79%)	61 (11%)	51 (10%)	1	3

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	4	ASP
1	B	90	LYS
1	B	96	GLY
1	B	113	GLN
1	B	114	TYR
1	B	115	PRO
1	B	117	ILE
1	B	134	ARG
1	B	136	ILE
1	B	168	GLU
1	B	209	ALA
1	B	210	LEU
1	A	90	LYS
1	A	103	LEU
1	A	146	ASP
1	A	172	PRO
1	A	195	THR
1	A	202	PRO
1	A	203	TRP
1	A	282	GLN
1	B	98	GLN
1	B	165	ARG
1	B	203	TRP
1	B	204	GLY
1	B	207	PHE

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Mol	Chain	Res	Type
1	B	208	TYR
1	B	281	HIS
1	A	88	GLU
1	A	244	LYS
1	B	30	THR
1	B	88	GLU
1	B	126	THR
1	B	282	GLN
1	A	142	SER
1	A	171	PRO
1	B	244	LYS
1	B	296	ARG
1	A	104	ILE
1	A	166	SER
1	A	169	ASP
1	A	176	MET
1	A	178	LEU
1	A	296	ARG
1	B	164	LYS
1	A	30	THR
1	A	89	GLY
1	A	139	LYS
1	A	193	SER
1	B	106	PHE
1	B	202	PRO
1	B	258	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	240/269 (89%)	199 (83%)	41 (17%)	2	10
1	B	245/269 (91%)	196 (80%)	49 (20%)	1	7
All	All	485/538 (90%)	395 (81%)	90 (19%)	2	9

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3	ASN
1	B	5	ILE
1	B	10	ARG
1	B	11	LEU
1	B	23	LEU
1	B	47	LYS
1	B	70	LEU
1	B	73	LYS
1	B	86	LEU
1	B	91	LEU
1	B	103	LEU
1	B	109	VAL
1	B	111	MET
1	B	112	GLU
1	B	116	TRP
1	B	117	ILE
1	B	128	LEU
1	B	133	LYS
1	B	134	ARG
1	B	153	PHE
1	B	158	LEU
1	B	164	LYS
1	B	174	HIS
1	B	175	ARG
1	B	177	GLU
1	B	184	GLU
1	B	188	ARG
1	B	189	ARG
1	B	198	ARG
1	B	199	ILE
1	B	207	PHE
1	B	208	TYR
1	B	211	THR
1	B	212	ARG
1	B	235	PHE
1	B	239	LYS
1	B	245	ARG
1	B	250	ARG
1	B	257	VAL
1	B	260	GLU
1	B	271	GLU
1	B	272	ILE
1	B	273	ILE

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Mol	Chain	Res	Type
1	B	274	ARG
1	B	275	THR
1	B	283	VAL
1	B	289	ILE
1	B	292	MET
1	B	297	LYS
1	A	5	ILE
1	A	11	LEU
1	A	23	LEU
1	A	47	LYS
1	A	70	LEU
1	A	86	LEU
1	A	91	LEU
1	A	97	SER
1	A	101	ARG
1	A	102	TYR
1	A	103	LEU
1	A	104	ILE
1	A	105	GLN
1	A	108	TYR
1	A	109	VAL
1	A	111	MET
1	A	139	LYS
1	A	144	LEU
1	A	152	SER
1	A	156	LEU
1	A	164	LYS
1	A	170	LEU
1	A	182	LEU
1	A	188	ARG
1	A	190	LEU
1	A	191	LEU
1	A	199	ILE
1	A	211	THR
1	A	235	PHE
1	A	239	LYS
1	A	250	ARG
1	A	255	LEU
1	A	257	VAL
1	A	260	GLU
1	A	271	GLU
1	A	272	ILE

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Mol	Chain	Res	Type
1	A	273	ILE
1	A	274	ARG
1	A	275	THR
1	A	292	MET
1	A	297	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	174	HIS
1	A	33	HIS
1	A	113	GLN

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

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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	272/307 (88%)	0.63	27 (9%) 9 5	41, 87, 157, 184	0
1	B	280/307 (91%)	0.54	12 (4%) 39 23	42, 90, 158, 178	0
2	C	21/21 (100%)	0.31	0 100 100	56, 75, 93, 99	0
3	D	21/21 (100%)	0.29	1 (4%) 34 20	52, 73, 98, 104	0
All	All	594/656 (90%)	0.57	40 (6%) 21 11	41, 87, 157, 184	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	259	PRO	8.6
1	A	141	PRO	6.7
1	A	176	MET	6.3
1	B	176	MET	5.9
1	B	203	TRP	4.1
1	B	116	TRP	3.8
1	A	260	GLU	3.8
1	A	6	ASP	3.4
1	A	258	PRO	3.3
1	B	106	PHE	3.3
1	A	88	GLU	3.2
1	A	262	TRP	3.1
1	A	143	ASN	3.1
1	A	192	TYR	3.1
1	A	174	HIS	3.0
1	B	108	TYR	2.7
1	B	10	ARG	2.7
1	B	97	SER	2.6
1	A	9	LYS	2.6
1	A	148	GLN	2.6
1	A	296	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	110	TRP	2.5
1	A	276	TRP	2.5
1	B	132	GLU	2.3
3	D	1	DA	2.3
1	A	142	SER	2.3
1	A	282	GLN	2.3
1	B	208	TYR	2.2
1	A	214	PHE	2.2
1	A	257	VAL	2.2
1	B	280	TYR	2.2
1	A	256	ASP	2.1
1	A	279	LYS	2.1
1	A	4	ASP	2.1
1	A	292	MET	2.1
1	A	173	GLU	2.1
1	A	115	PRO	2.1
1	A	265	ALA	2.1
1	B	276	TRP	2.0
1	A	87	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	CA	C	102	1/1	0.92	0.39	-	105,105,105,105	0
4	CA	C	101	1/1	0.57	0.86	-	105,105,105,105	0
4	CA	D	101	1/1	0.87	0.41	-	110,110,110,110	0

6.5 Other polymers [i](#)

There are no such residues in this entry.