



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:04 PM UTC

PDB ID : 5HBU / pdb_00005hbu
Title : Structure of the E. coli nucleoid occlusion protein SlmA bound to DNA and the C-terminal tail of the cytoskeletal cell division protein FtsZ
Authors : Schumacher, M.A.; Zeng, W.
Deposited on : 2016-01-02
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

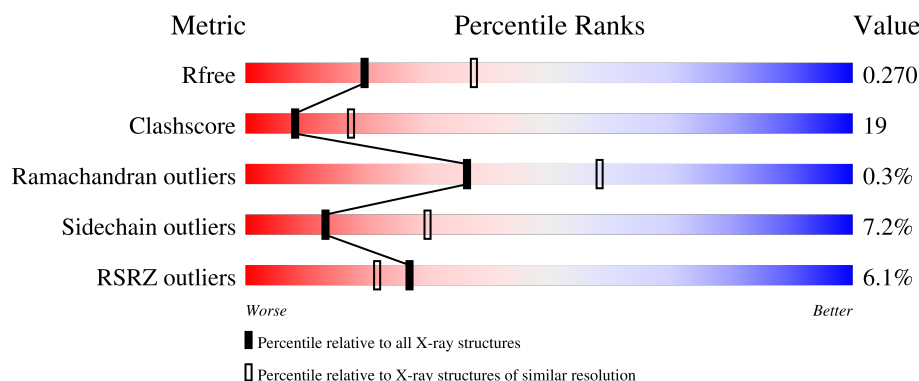
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



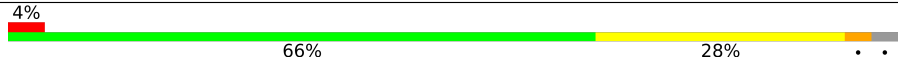
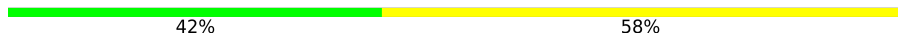
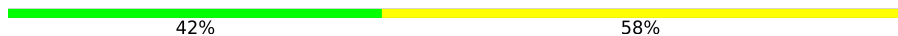
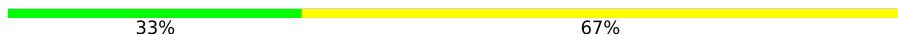
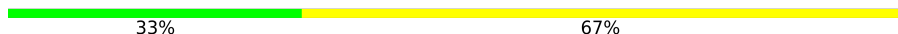
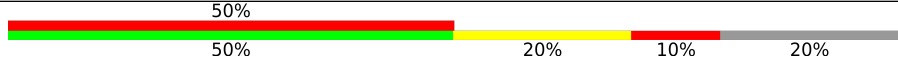
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	196	13% 53% 40% • •
1	B	196	15% 59% 35% 6% • •
1	C	196	2% 62% 33% • •
1	D	196	4% 62% 30% • •
1	E	196	4% 59% 34% • •

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Mol	Chain	Length	Quality of chain
1	F	196	
1	G	196	
1	H	196	
2	R	12	
2	T	12	
2	W	12	
2	Z	12	
3	K	10	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13710 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 Nucleoid occlusion factor SlmA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	190	Total	C	N	O	S	0	0	0
			1543	970	281	286	6			
1	B	196	Total	C	N	O	S	0	0	0
			1589	998	290	295	6			
1	C	190	Total	C	N	O	S	0	0	0
			1543	970	281	286	6			
1	D	189	Total	C	N	O	S	0	0	0
			1532	964	277	285	6			
1	E	190	Total	C	N	O	S	0	0	0
			1543	970	281	286	6			
1	F	189	Total	C	N	O	S	0	0	0
			1532	964	277	285	6			
1	G	190	Total	C	N	O	S	0	0	0
			1543	970	281	286	6			
1	H	190	Total	C	N	O	S	0	0	0
			1543	970	281	286	6			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ALA	-	expression tag	UNP P0C093
A	4	GLU	-	expression tag	UNP P0C093
A	5	LYS	-	expression tag	UNP P0C093
A	6	GLN	-	expression tag	UNP P0C093
B	3	ALA	-	expression tag	UNP P0C093
B	4	GLU	-	expression tag	UNP P0C093
B	5	LYS	-	expression tag	UNP P0C093
B	6	GLN	-	expression tag	UNP P0C093
C	3	ALA	-	expression tag	UNP P0C093
C	4	GLU	-	expression tag	UNP P0C093
C	5	LYS	-	expression tag	UNP P0C093
C	6	GLN	-	expression tag	UNP P0C093
D	3	ALA	-	expression tag	UNP P0C093

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Chain	Residue	Modelled	Actual	Comment	Reference
D	4	GLU	-	expression tag	UNP P0C093
D	5	LYS	-	expression tag	UNP P0C093
D	6	GLN	-	expression tag	UNP P0C093
E	3	ALA	-	expression tag	UNP P0C093
E	4	GLU	-	expression tag	UNP P0C093
E	5	LYS	-	expression tag	UNP P0C093
E	6	GLN	-	expression tag	UNP P0C093
F	3	ALA	-	expression tag	UNP P0C093
F	4	GLU	-	expression tag	UNP P0C093
F	5	LYS	-	expression tag	UNP P0C093
F	6	GLN	-	expression tag	UNP P0C093
G	3	ALA	-	expression tag	UNP P0C093
G	4	GLU	-	expression tag	UNP P0C093
G	5	LYS	-	expression tag	UNP P0C093
G	6	GLN	-	expression tag	UNP P0C093
H	3	ALA	-	expression tag	UNP P0C093
H	4	GLU	-	expression tag	UNP P0C093
H	5	LYS	-	expression tag	UNP P0C093
H	6	GLN	-	expression tag	UNP P0C093

- Molecule 2 is a DNA chain called DNA (5'-D(*GP*TP*GP*AP*GP*TP*AP*CP*TP*CP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	12	Total	C	N	O	P	0	0	0
			243	117	45	70	11			
2	Z	12	Total	C	N	O	P	0	0	0
			243	117	45	70	11			
2	R	12	Total	C	N	O	P	0	0	0
			243	117	45	70	11			
2	T	12	Total	C	N	O	P	0	0	0
			243	117	45	70	11			

- Molecule 3 is a protein called FtsZ CTT peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	K	8	Total	C	N	O	0	0	0
			67	45	11	11			

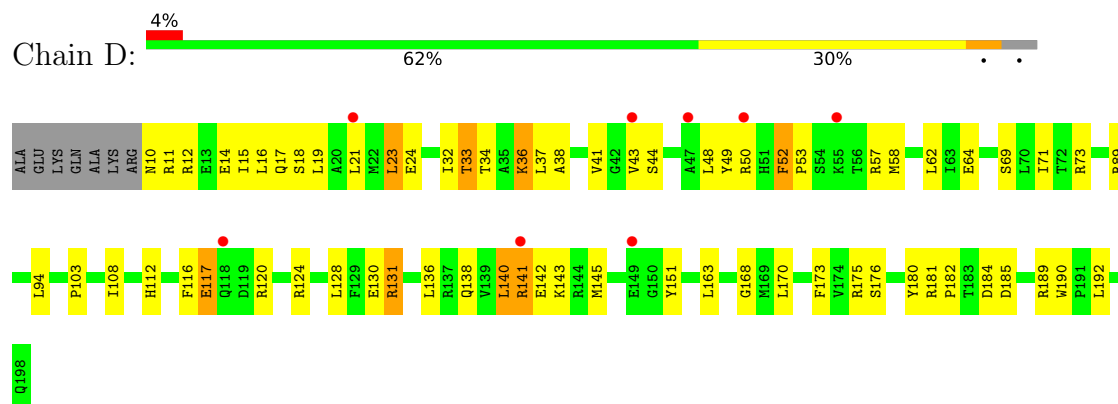
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	17	Total 17	O 17	0	0
4	B	10	Total 10	O 10	0	0
4	C	58	Total 58	O 58	0	0
4	D	48	Total 48	O 48	0	0
4	E	28	Total 28	O 28	0	0
4	F	29	Total 29	O 29	0	0
4	G	50	Total 50	O 50	0	0
4	H	36	Total 36	O 36	0	0
4	W	9	Total 9	O 9	0	0
4	Z	7	Total 7	O 7	0	0
4	R	7	Total 7	O 7	0	0
4	T	2	Total 2	O 2	0	0
4	K	2	Total 2	O 2	0	0

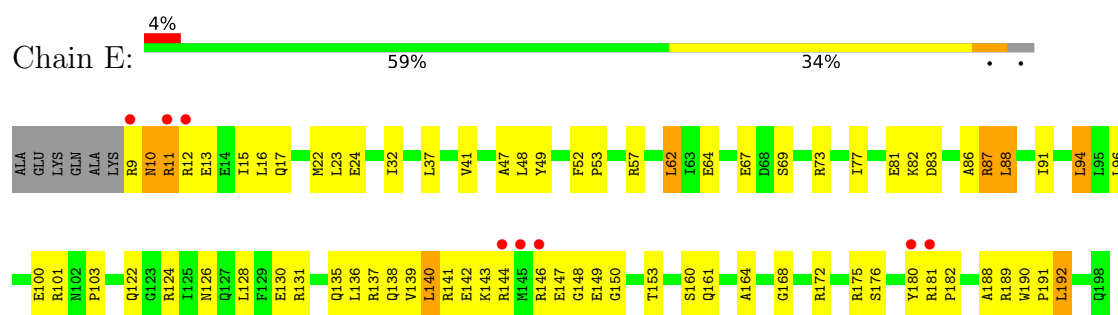
- Molecule 1: Nucleoid occlusion factor SlmA



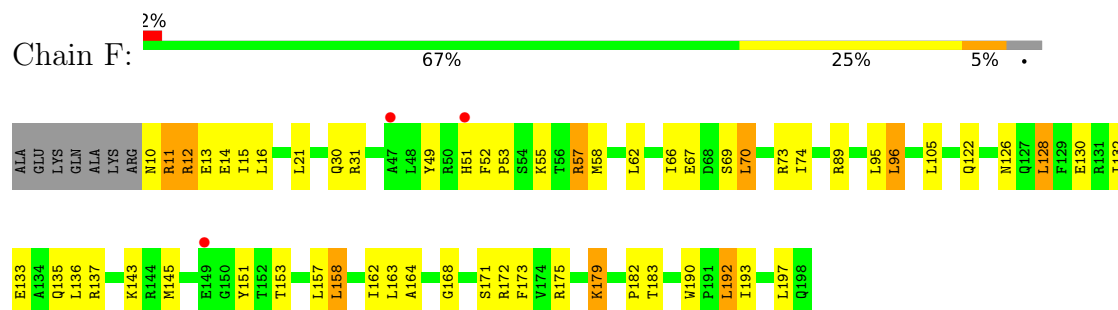
- Molecule 1: Nucleoid occlusion factor SlmA



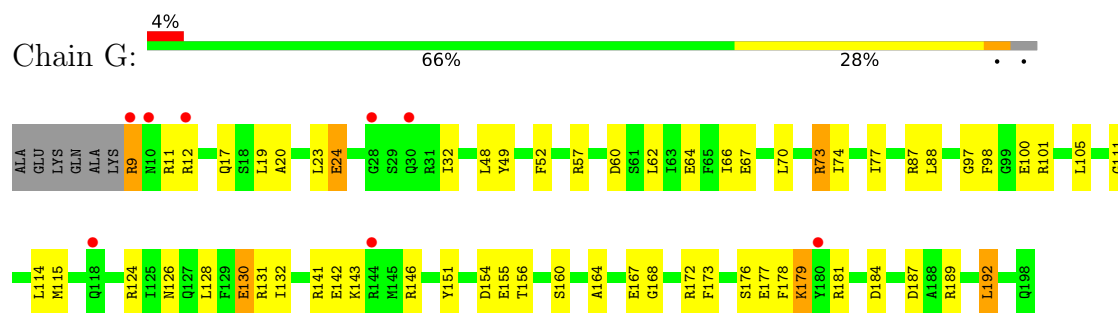
- Molecule 1: Nucleoid occlusion factor SlmA



- Molecule 1: Nucleoid occlusion factor SlmA

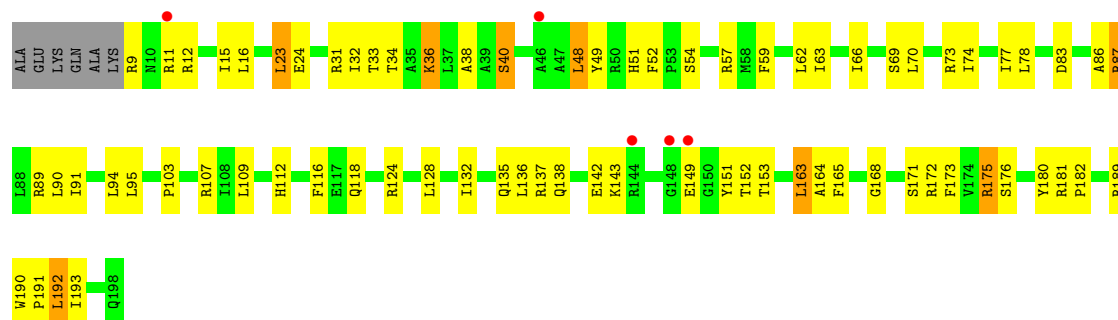


- Molecule 1: Nucleoid occlusion factor SlmA



- Molecule 1: Nucleoid occlusion factor SlmA

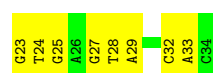




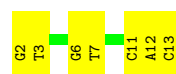
- Molecule 2: DNA (5'-D(*GP*TP*GP*AP*GP*TP*AP*CP*TP*CP*AP*C)-3')



- Molecule 2: DNA (5'-D(*GP*TP*GP*AP*GP*TP*AP*CP*TP*CP*AP*C)-3')



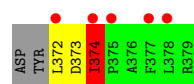
- Molecule 2: DNA (5'-D(*GP*TP*GP*AP*GP*TP*AP*CP*TP*CP*AP*C)-3')



- Molecule 2: DNA (5'-D(*GP*TP*GP*AP*GP*TP*AP*CP*TP*CP*AP*C)-3')



- Molecule 3: FtsZ CTT peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.11Å 158.89Å 200.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.10 – 2.60 100.10 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (100.10-2.60) 99.7 (100.10-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.62Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.226 , 0.270 0.226 , 0.270	Depositor DCC
R_{free} test set	2000 reflections (2.87%)	wwPDB-VP
Wilson B-factor (Å ²)	37.3	Xtriage
Anisotropy	0.808	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13710	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.13 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.2397e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.30	0/1563	0.75	2/2098 (0.1%)
1	B	0.30	0/1609	0.77	1/2158 (0.0%)
1	C	0.27	0/1563	0.70	2/2098 (0.1%)
1	D	0.32	0/1552	0.74	2/2084 (0.1%)
1	E	0.28	0/1563	0.69	0/2098
1	F	0.27	0/1552	0.71	0/2084
1	G	0.27	0/1563	0.74	0/2098
1	H	0.28	0/1563	0.71	2/2098 (0.1%)
2	R	0.11	0/272	0.53	0/418
2	T	0.07	0/272	0.53	0/418
2	W	0.09	0/272	0.53	0/418
2	Z	0.09	0/272	0.55	0/418
3	K	0.24	0/68	0.98	2/90 (2.2%)
All	All	0.28	0/13684	0.71	11/18578 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	51	HIS	N-CA-C	-5.77	107.48	114.75
1	H	181	ARG	CA-C-N	5.65	125.76	119.32
1	H	181	ARG	C-N-CA	5.65	125.76	119.32
1	A	181	ARG	CA-C-N	5.38	125.71	119.47
1	A	181	ARG	C-N-CA	5.38	125.71	119.47
1	D	52	PHE	CA-C-N	5.22	124.83	119.56
1	D	52	PHE	C-N-CA	5.22	124.83	119.56
3	K	374	ILE	CA-C-N	5.15	124.91	119.76
3	K	374	ILE	C-N-CA	5.15	124.91	119.76
1	C	181	ARG	CA-C-N	5.02	124.80	119.28
1	C	181	ARG	C-N-CA	5.02	124.80	119.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1543	0	1579	85	0
1	B	1589	0	1629	89	0
1	C	1543	0	1579	60	0
1	D	1532	0	1566	68	0
1	E	1543	0	1579	69	0
1	F	1532	0	1566	48	0
1	G	1543	0	1579	49	0
1	H	1543	0	1579	62	0
2	R	243	0	137	9	0
2	T	243	0	137	8	0
2	W	243	0	137	6	0
2	Z	243	0	137	13	0
3	K	67	0	70	3	0
4	A	17	0	0	10	0
4	B	10	0	0	1	0
4	C	58	0	0	7	0
4	D	48	0	0	3	0
4	E	28	0	0	3	0
4	F	29	0	0	1	0
4	G	50	0	0	4	0
4	H	36	0	0	2	0
4	K	2	0	0	0	0
4	R	7	0	0	2	0
4	T	2	0	0	0	0
4	W	9	0	0	0	0
4	Z	7	0	0	0	0
All	All	13710	0	13274	517	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 19.

All (517) 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:A:140:LEU:CD2	1:A:158:LEU:HD11	1.75	1.16
1:D:36:LYS:HB2	1:D:36:LYS:HZ3	1.00	1.16
1:A:140:LEU:HD21	1:A:158:LEU:CD1	1.86	1.05
1:D:64:GLU:HG3	1:D:124:ARG:HH22	1.25	1.01
1:C:73:ARG:HH12	1:C:101:ARG:HH12	1.07	1.00
1:D:37:LEU:HD21	1:D:58:MET:HE1	1.45	0.98
1:D:36:LYS:HB2	1:D:36:LYS:NZ	1.78	0.98
1:A:140:LEU:HD21	1:A:158:LEU:HD11	0.97	0.96
2:T:27:DG:H2''	2:T:28:DT:H5'	1.47	0.96
1:D:33:THR:OG1	1:D:36:LYS:NZ	2.00	0.94
1:B:77:ILE:HD11	1:B:90:LEU:CB	1.97	0.93
1:B:77:ILE:HD11	1:B:90:LEU:HB3	1.51	0.92
1:C:67:GLU:HG2	1:C:128:LEU:HD13	1.52	0.91
1:B:66:ILE:HG22	1:B:98:PHE:HZ	1.40	0.87
1:G:67:GLU:HG3	1:G:128:LEU:HD13	1.56	0.87
1:E:82:LYS:HB3	1:E:146:ARG:NH2	1.90	0.86
1:G:130:GLU:HG2	4:H:206:HOH:O	1.76	0.86
1:A:64:GLU:HG2	1:A:124:ARG:HH22	1.40	0.86
1:B:93:LEU:HB2	1:B:186:PHE:CE2	2.12	0.85
1:B:74:ILE:O	1:B:77:ILE:HG22	1.78	0.83
1:D:33:THR:HG22	2:Z:33:DA:P	2.19	0.82
2:W:2:DG:H2'	2:W:3:DT:H71	1.63	0.81
1:A:10:ASN:O	1:A:14:GLU:HB2	1.81	0.81
1:E:88:LEU:HD21	1:E:140:LEU:HD11	1.61	0.80
1:D:17:GLN:O	1:D:21:LEU:HD12	1.80	0.80
1:G:167:GLU:OE1	1:H:172:ARG:HG2	1.82	0.79
1:B:13:GLU:O	1:B:17:GLN:HG2	1.81	0.79
1:G:73:ARG:HH21	1:G:101:ARG:NH2	1.81	0.79
1:G:111:GLY:O	4:G:201:HOH:O	2.01	0.78
1:B:66:ILE:HG22	1:B:98:PHE:CZ	2.17	0.78
1:G:64:GLU:HG3	1:G:124:ARG:HH22	1.47	0.78
1:G:141:ARG:HD3	4:G:238:HOH:O	1.83	0.78
1:B:32:ILE:HA	1:B:36:LYS:HE2	1.66	0.77
1:B:78:LEU:HD21	1:B:135:GLN:OE1	1.84	0.77
1:D:69:SER:O	1:D:73:ARG:HG2	1.84	0.76
1:B:16:LEU:HD11	1:B:52:PHE:CZ	2.20	0.76
1:B:73:ARG:HB3	1:B:94:LEU:HD21	1.68	0.75
1:H:12:ARG:HG3	1:H:51:HIS:HB3	1.68	0.75
1:H:77:ILE:HG21	1:H:91:ILE:CD1	2.17	0.74
1:E:142:GLU:O	1:E:146:ARG:HG3	1.87	0.74
1:B:16:LEU:HD11	1:B:52:PHE:HZ	1.53	0.73
1:E:12:ARG:HH22	1:E:16:LEU:HD11	1.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:91:ILE:HG21	1:H:136:LEU:HD11	1.68	0.73
1:A:192:LEU:HD11	1:B:153:THR:HG21	1.70	0.73
1:A:71:ILE:HD11	1:A:131:ARG:HG2	1.71	0.73
1:C:64:GLU:HG3	1:C:124:ARG:HH22	1.54	0.72
1:G:142:GLU:HG2	1:G:146:ARG:HE	1.54	0.72
1:E:64:GLU:HG3	1:E:124:ARG:HH22	1.54	0.72
1:B:77:ILE:CD1	1:B:90:LEU:HB3	2.19	0.72
1:B:63:ILE:O	1:B:66:ILE:HG13	1.90	0.72
1:D:36:LYS:HZ3	1:D:36:LYS:CB	1.88	0.72
1:E:64:GLU:CG	1:E:124:ARG:HH22	2.03	0.72
1:H:49:TYR:CE1	2:R:13:DC:H2'	2.25	0.72
1:A:49:TYR:HD2	4:A:201:HOH:O	1.74	0.71
1:A:56:THR:HG21	1:A:118:GLN:OE1	1.90	0.71
1:A:163:LEU:HD23	1:B:172:ARG:HH12	1.56	0.71
1:A:158:LEU:C	1:A:158:LEU:HD12	2.16	0.71
1:G:181:ARG:HB2	1:G:184:ASP:CG	2.16	0.71
1:B:77:ILE:HD11	1:B:90:LEU:HB2	1.71	0.70
1:D:33:THR:CG2	2:Z:32:DC:H3'	2.22	0.70
1:A:46:ALA:HA	4:A:201:HOH:O	1.92	0.69
1:D:143:LYS:HD2	1:D:151:TYR:CZ	2.26	0.69
1:D:120:ARG:HG2	1:D:120:ARG:HH11	1.57	0.69
1:A:64:GLU:HG2	1:A:124:ARG:NH2	2.07	0.69
1:D:64:GLU:HG3	1:D:124:ARG:NH2	2.04	0.68
1:F:55:LYS:HA	1:F:58:MET:HE3	1.75	0.68
1:C:131:ARG:NE	4:C:203:HOH:O	2.25	0.68
1:B:12:ARG:HG2	1:B:13:GLU:N	2.08	0.68
1:B:191:PRO:HG2	1:B:192:LEU:HD12	1.74	0.68
1:G:126:ASN:OD1	1:H:175:ARG:HD2	1.94	0.68
1:A:60:ASP:O	1:A:64:GLU:HG3	1.93	0.68
1:A:151:TYR:HD1	1:A:198:GLN:OXT	1.76	0.67
1:B:9:ARG:CD	1:B:12:ARG:HD2	2.24	0.67
2:R:6:DG:H4'	2:R:7:DT:OP1	1.94	0.67
1:D:15:ILE:HD11	1:D:52:PHE:CE2	2.30	0.66
1:C:9:ARG:NH1	1:C:10:ASN:HB2	2.10	0.66
4:C:255:HOH:O	1:D:175:ARG:HG3	1.96	0.66
1:A:49:TYR:HA	1:A:52:PHE:O	1.96	0.65
1:E:160:SER:HB2	1:F:172:ARG:HH12	1.62	0.65
1:A:141:ARG:HG2	1:A:155:GLU:HG2	1.76	0.65
1:B:95:LEU:HD21	1:B:132:ILE:HD13	1.78	0.65
1:E:9:ARG:C	1:E:11:ARG:H	2.05	0.65
1:D:15:ILE:CD1	1:D:52:PHE:CE2	2.80	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:ASN:O	4:C:201:HOH:O	2.13	0.65
1:D:138:GLN:OE1	1:D:142:GLU:OE1	2.15	0.65
1:E:88:LEU:HD21	1:E:140:LEU:CD1	2.26	0.65
1:B:109:LEU:O	4:B:201:HOH:O	2.14	0.65
1:A:79:LYS:HG3	1:A:80:ASP:OD1	1.97	0.65
1:H:77:ILE:HG21	1:H:91:ILE:HD12	1.78	0.65
2:R:11:DC:OP2	4:R:101:HOH:O	2.14	0.65
1:B:32:ILE:HA	1:B:36:LYS:CE	2.26	0.65
1:G:73:ARG:HH21	1:G:101:ARG:HH22	1.45	0.64
1:A:83:ASP:HB3	1:A:86:ALA:HB3	1.77	0.64
1:D:12:ARG:O	1:D:15:ILE:HG13	1.96	0.64
1:C:51:HIS:CD2	4:C:207:HOH:O	2.51	0.64
1:F:143:LYS:HD2	1:F:151:TYR:CZ	2.33	0.64
1:G:160:SER:HB2	1:H:172:ARG:HH12	1.63	0.63
1:C:144:ARG:NH1	1:C:145:MET:HE3	2.13	0.63
1:E:53:PRO:HG2	1:E:57:ARG:HG3	1.78	0.63
1:A:158:LEU:HD12	1:A:159:ALA:N	2.14	0.63
1:D:116:PHE:C	1:D:117:GLU:OE2	2.42	0.62
1:D:23:LEU:HD13	1:D:32:ILE:HD12	1.81	0.62
1:B:9:ARG:HD3	1:B:12:ARG:HD2	1.80	0.62
1:C:73:ARG:HH12	1:C:101:ARG:NH1	1.89	0.62
1:B:183:THR:HG22	1:B:183:THR:O	2.00	0.62
1:D:117:GLU:N	1:D:117:GLU:CD	2.57	0.62
1:G:115:MET:HE3	1:H:112:HIS:CD2	2.35	0.62
1:A:27:ASP:OD2	1:E:141:ARG:NH2	2.33	0.62
1:F:73:ARG:O	3:K:372:LEU:HD21	1.99	0.62
1:H:23:LEU:HD13	1:H:32:ILE:HD11	1.82	0.62
1:C:17:GLN:O	1:C:21:LEU:HG	2.00	0.61
1:F:11:ARG:HA	1:F:14:GLU:OE2	2.00	0.61
1:B:43:VAL:HG22	1:B:44:SER:H	1.65	0.61
1:B:181:ARG:O	1:B:184:ASP:HB2	2.00	0.61
1:F:179:LYS:NZ	2:Z:27:DG:OP2	2.33	0.61
1:A:157:LEU:O	1:A:157:LEU:HG	2.00	0.61
1:D:64:GLU:CG	1:D:124:ARG:HH22	2.09	0.61
1:F:11:ARG:HA	1:F:14:GLU:HG2	1.82	0.61
1:F:96:LEU:HB3	1:F:183:THR:HG22	1.83	0.61
1:A:64:GLU:CG	1:A:124:ARG:HH22	2.11	0.61
1:B:66:ILE:HD13	1:B:109:LEU:HD21	1.82	0.61
1:F:89:ARG:HB2	1:F:190:TRP:CZ2	2.36	0.60
1:G:167:GLU:OE1	1:H:172:ARG:CG	2.49	0.60
1:F:173:PHE:CD1	1:F:182:PRO:HD3	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ARG:HB3	1:B:94:LEU:CD2	2.31	0.60
1:C:97:GLY:O	1:C:101:ARG:HG2	2.01	0.60
1:E:83:ASP:HB3	1:E:86:ALA:HB3	1.83	0.60
1:F:53:PRO:HD2	1:F:57:ARG:HG3	1.83	0.60
1:D:33:THR:HG22	2:Z:32:DC:H3'	1.82	0.59
1:B:33:THR:OG1	1:B:36:LYS:HG2	2.03	0.59
1:D:38:ALA:HB1	1:D:43:VAL:O	2.01	0.59
1:D:140:LEU:HD12	1:D:151:TYR:CE2	2.37	0.59
1:G:20:ALA:O	1:G:24:GLU:HB2	2.01	0.59
1:A:91:ILE:HG21	1:A:136:LEU:HD11	1.82	0.59
1:B:9:ARG:HA	1:B:12:ARG:HB3	1.83	0.59
1:C:73:ARG:NH1	1:C:101:ARG:HH12	1.90	0.59
1:A:76:LEU:O	1:A:79:LYS:HG2	2.02	0.59
1:A:196:GLN:HG2	1:B:192:LEU:O	2.02	0.59
1:D:130:GLU:OE2	4:D:201:HOH:O	2.17	0.58
1:E:12:ARG:HG2	1:E:12:ARG:HH21	1.66	0.58
1:A:137:ARG:HD2	1:A:141:ARG:HH22	1.68	0.58
1:D:24:GLU:HG3	1:D:103:PRO:HB2	1.84	0.58
1:D:37:LEU:O	1:D:41:VAL:HG23	2.03	0.58
2:R:6:DG:H2''	2:R:7:DT:O5'	2.03	0.58
1:C:64:GLU:HG3	1:C:124:ARG:NH2	2.16	0.58
1:D:33:THR:HG21	2:Z:32:DC:H3'	1.85	0.58
1:G:141:ARG:HB3	1:G:155:GLU:HG2	1.84	0.58
1:D:141:ARG:NH2	4:D:208:HOH:O	2.36	0.58
1:B:190:TRP:N	1:B:191:PRO:HD2	2.18	0.57
1:A:95:LEU:HD21	1:A:132:ILE:HD13	1.86	0.57
1:H:168:GLY:O	1:H:172:ARG:HG3	2.03	0.57
1:E:172:ARG:HH12	1:F:163:LEU:HD23	1.69	0.57
1:H:171:SER:O	1:H:175:ARG:HB2	2.05	0.57
1:A:87:ARG:HD3	1:A:139:VAL:HG13	1.86	0.57
1:D:11:ARG:NH2	4:D:210:HOH:O	2.37	0.57
1:A:181:ARG:NH2	1:E:148:GLY:O	2.37	0.57
1:C:173:PHE:CD1	1:C:182:PRO:HD3	2.40	0.57
1:G:173:PHE:CE1	1:G:178:PHE:HA	2.40	0.57
1:A:118:GLN:HG3	4:A:205:HOH:O	2.04	0.57
1:A:26:SER:HA	4:A:213:HOH:O	2.04	0.57
1:E:24:GLU:HG3	1:E:103:PRO:HB2	1.87	0.57
1:A:192:LEU:O	1:B:196:GLN:HG2	2.05	0.57
1:C:74:ILE:HG21	1:C:135:GLN:HG2	1.87	0.57
1:G:97:GLY:O	1:G:101:ARG:HG2	2.04	0.57
1:F:11:ARG:HA	1:F:14:GLU:CG	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ARG:HG2	1:B:94:LEU:HD13	1.88	0.56
1:D:15:ILE:HG13	1:D:16:LEU:H	1.71	0.56
1:E:136:LEU:O	1:E:140:LEU:HD22	2.06	0.56
1:B:49:TYR:HA	1:B:52:PHE:O	2.06	0.56
1:A:181:ARG:NH2	1:E:144:ARG:NH2	2.53	0.56
1:D:43:VAL:HG12	1:D:44:SER:N	2.21	0.56
1:F:168:GLY:O	1:F:172:ARG:HG3	2.05	0.56
1:B:21:LEU:O	1:B:21:LEU:HD12	2.06	0.56
2:T:26:DA:H2''	2:T:27:DG:O5'	2.06	0.56
1:C:19:LEU:HD13	1:C:62:LEU:HD22	1.88	0.55
1:H:23:LEU:O	1:H:107:ARG:HD2	2.07	0.55
2:W:6:DG:H4'	2:W:7:DT:OP1	2.06	0.55
1:A:146:ARG:NH2	4:A:202:HOH:O	2.39	0.55
1:H:33:THR:OG1	1:H:36:LYS:HB2	2.06	0.55
2:T:27:DG:H2''	2:T:28:DT:C5'	2.31	0.55
1:A:151:TYR:CD1	1:A:198:GLN:OXT	2.59	0.55
1:B:19:LEU:O	1:B:19:LEU:HD12	2.07	0.55
1:B:100:GLU:HB2	1:B:182:PRO:HG2	1.89	0.55
1:C:83:ASP:OD2	4:C:202:HOH:O	2.17	0.55
1:G:173:PHE:CD1	1:G:178:PHE:HA	2.42	0.55
1:H:49:TYR:HE1	2:R:13:DC:H2'	1.69	0.55
1:C:11:ARG:O	1:C:15:ILE:HG13	2.07	0.55
1:B:89:ARG:HH11	1:B:190:TRP:CD1	2.25	0.55
1:F:12:ARG:HG3	1:F:51:HIS:HB3	1.88	0.54
1:A:73:ARG:HB2	1:A:94:LEU:HD21	1.89	0.54
1:D:117:GLU:OE2	1:D:117:GLU:N	2.41	0.54
1:F:95:LEU:HD21	1:F:132:ILE:HD13	1.89	0.54
1:C:115:MET:HE3	1:D:112:HIS:HB3	1.90	0.54
1:E:137:ARG:O	1:E:141:ARG:HG3	2.07	0.54
1:A:57:ARG:HA	1:A:60:ASP:HB2	1.89	0.54
1:C:143:LYS:HD2	1:C:151:TYR:CZ	2.43	0.54
1:H:78:LEU:HD23	1:H:87:ARG:HG2	1.90	0.54
2:T:27:DG:C2'	2:T:28:DT:H5'	2.31	0.54
1:A:91:ILE:HG21	1:A:136:LEU:CD1	2.37	0.54
1:E:49:TYR:HA	1:E:52:PHE:O	2.08	0.54
1:H:69:SER:O	1:H:73:ARG:HG2	2.08	0.54
1:C:137:ARG:HG2	1:C:141:ARG:NH1	2.22	0.54
1:G:57:ARG:NE	4:G:206:HOH:O	2.41	0.54
1:D:173:PHE:CD1	1:D:182:PRO:HD3	2.42	0.53
1:H:66:ILE:HG21	1:H:109:LEU:HD21	1.90	0.53
1:A:89:ARG:HH11	1:A:190:TRP:CD1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:173:PHE:CD1	1:H:182:PRO:HD3	2.43	0.53
1:A:72:THR:HG22	1:A:73:ARG:N	2.23	0.53
1:E:67:GLU:HG3	1:E:128:LEU:HD13	1.90	0.53
1:G:178:PHE:O	1:G:181:ARG:NH1	2.36	0.53
1:C:141:ARG:HD3	4:C:244:HOH:O	2.08	0.53
1:C:115:MET:HE3	1:D:112:HIS:CD2	2.43	0.53
1:H:24:GLU:HG3	1:H:103:PRO:HB2	1.91	0.53
1:E:144:ARG:HA	1:E:149:GLU:O	2.08	0.53
2:W:6:DG:H2''	2:W:7:DT:O5'	2.07	0.53
1:A:141:ARG:CG	1:A:155:GLU:HG2	2.38	0.53
1:E:9:ARG:NH1	1:E:10:ASN:OD1	2.42	0.53
1:E:91:ILE:HG21	1:E:136:LEU:HD11	1.91	0.53
1:D:33:THR:HG22	2:Z:33:DA:OP1	2.08	0.53
1:E:69:SER:O	1:E:73:ARG:HG3	2.09	0.53
1:E:175:ARG:HB2	1:F:122:GLN:NE2	2.23	0.53
1:B:49:TYR:CE1	2:W:13:DC:H2'	2.43	0.52
1:H:78:LEU:HD11	1:H:135:GLN:CD	2.34	0.52
1:B:175:ARG:C	1:B:177:GLU:H	2.16	0.52
1:A:129:PHE:CG	1:B:175:ARG:NH2	2.77	0.52
1:A:132:ILE:O	1:A:136:LEU:HB2	2.09	0.52
1:C:49:TYR:OH	2:W:8:DA:H2''	2.09	0.52
1:E:160:SER:HB2	1:F:172:ARG:NH1	2.23	0.52
1:C:31:ARG:NH1	1:C:116:PHE:HB3	2.24	0.52
1:G:57:ARG:HA	1:G:60:ASP:HB2	1.91	0.52
1:A:168:GLY:O	1:A:172:ARG:HG3	2.09	0.52
1:D:36:LYS:NZ	1:D:36:LYS:CB	2.54	0.52
1:A:67:GLU:O	1:A:71:ILE:HB	2.10	0.51
1:B:63:ILE:CG2	1:B:124:ARG:HE	2.24	0.51
1:G:70:LEU:HD23	1:G:132:ILE:HD11	1.92	0.51
1:A:153:THR:HG21	1:B:192:LEU:HD21	1.92	0.51
1:A:31:ARG:HB3	1:A:116:PHE:CD2	2.45	0.51
1:E:81:GLU:O	1:E:87:ARG:HD2	2.11	0.51
1:F:74:ILE:HG21	1:F:135:GLN:HG2	1.93	0.51
1:A:19:LEU:O	1:A:23:LEU:HD13	2.11	0.51
1:D:15:ILE:HD11	1:D:52:PHE:CZ	2.46	0.51
1:C:31:ARG:HH11	1:C:116:PHE:HB3	1.76	0.51
1:E:188:ALA:N	4:E:206:HOH:O	2.44	0.51
1:E:175:ARG:HB2	1:F:122:GLN:HE21	1.75	0.51
1:H:33:THR:HG22	2:R:11:DC:H3'	1.92	0.51
1:A:133:GLU:HB2	1:A:163:LEU:HD22	1.93	0.50
1:A:173:PHE:CD1	1:A:182:PRO:HD3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:THR:H	1:B:36:LYS:HE2	1.77	0.50
1:E:13:GLU:O	1:E:17:GLN:HG2	2.12	0.50
1:F:69:SER:O	1:F:73:ARG:HD3	2.11	0.50
1:F:133:GLU:HB2	1:F:163:LEU:HD22	1.91	0.50
1:A:45:GLU:O	1:A:48:LEU:HB2	2.11	0.50
1:B:89:ARG:NH1	1:B:190:TRP:CD1	2.79	0.50
1:E:12:ARG:NH2	1:E:16:LEU:HD11	2.22	0.50
1:B:192:LEU:HD12	1:B:192:LEU:H	1.77	0.50
1:D:33:THR:HG1	1:D:36:LYS:NZ	2.06	0.50
1:G:168:GLY:HA3	1:H:164:ALA:O	2.11	0.50
1:H:87:ARG:O	1:H:91:ILE:HD13	2.12	0.50
1:B:117:GLU:HB3	1:B:121:LEU:HD12	1.94	0.50
1:C:71:ILE:HG21	1:C:131:ARG:NH2	2.26	0.50
1:C:181:ARG:HB2	1:C:184:ASP:CG	2.37	0.50
1:D:181:ARG:HB2	1:D:184:ASP:OD2	2.11	0.50
2:R:11:DC:H2''	2:R:12:DA:C8	2.47	0.49
1:F:31:ARG:NH2	4:F:201:HOH:O	2.21	0.49
1:G:168:GLY:O	1:G:172:ARG:HG3	2.11	0.49
2:Z:24:DT:H2''	2:Z:25:DG:C8	2.46	0.49
1:D:181:ARG:O	1:D:184:ASP:HB2	2.11	0.49
1:G:98:PHE:HA	1:G:101:ARG:CZ	2.43	0.49
1:A:24:GLU:HB2	1:A:103:PRO:HB2	1.94	0.49
1:B:87:ARG:O	1:B:91:ILE:HG13	2.13	0.49
1:C:51:HIS:NE2	4:C:207:HOH:O	2.34	0.49
2:T:23:DG:H2''	2:T:24:DT:H5'	1.93	0.49
1:D:15:ILE:HG13	1:D:16:LEU:N	2.27	0.49
1:E:176:SER:CB	1:E:180:TYR:HD2	2.25	0.49
1:E:189:ARG:O	1:E:192:LEU:HB2	2.12	0.49
1:F:70:LEU:HD23	1:F:132:ILE:HD11	1.94	0.49
1:C:24:GLU:HG3	1:C:103:PRO:HB2	1.93	0.49
1:E:168:GLY:HA3	1:F:164:ALA:O	2.12	0.49
1:F:66:ILE:HD11	1:F:105:LEU:HB3	1.94	0.49
1:A:185:ASP:O	1:A:189:ARG:HG3	2.12	0.49
1:H:77:ILE:HG21	1:H:91:ILE:HD11	1.95	0.49
1:A:70:LEU:O	1:A:74:ILE:HG12	2.13	0.48
1:F:158:LEU:HD21	1:F:197:LEU:HD23	1.95	0.48
1:B:9:ARG:HD2	1:B:12:ARG:HD2	1.94	0.48
1:E:12:ARG:HG2	1:E:12:ARG:NH2	2.29	0.48
1:E:82:LYS:O	1:E:146:ARG:NE	2.45	0.48
1:C:9:ARG:HG3	1:C:10:ASN:N	2.26	0.48
1:D:189:ARG:O	1:D:192:LEU:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ALA:CA	4:A:201:HOH:O	2.56	0.48
1:A:49:TYR:CD2	4:A:201:HOH:O	2.55	0.48
1:B:165:PHE:CE2	1:B:193:ILE:HD11	2.49	0.48
1:E:77:ILE:HG22	1:E:87:ARG:HG3	1.95	0.48
1:B:12:ARG:O	1:B:15:ILE:N	2.32	0.48
1:F:49:TYR:CE1	2:T:34:DC:H2'	2.49	0.48
1:H:12:ARG:HG2	1:H:52:PHE:CZ	2.49	0.48
1:F:11:ARG:O	1:F:15:ILE:HG12	2.14	0.48
1:G:49:TYR:HA	1:G:52:PHE:O	2.14	0.48
1:G:176:SER:O	1:G:179:LYS:HG3	2.14	0.48
1:A:137:ARG:HD2	1:A:141:ARG:NH2	2.29	0.48
1:C:142:GLU:HA	1:C:145:MET:SD	2.54	0.48
1:H:189:ARG:O	1:H:192:LEU:HB2	2.14	0.48
1:C:135:GLN:O	1:C:139:VAL:HG23	2.14	0.47
1:E:67:GLU:CG	1:E:128:LEU:HD13	2.44	0.47
1:B:93:LEU:HB2	1:B:186:PHE:HE2	1.70	0.47
1:F:16:LEU:HD22	1:F:62:LEU:HD13	1.96	0.47
1:H:149:GLU:CD	1:H:149:GLU:H	2.21	0.47
1:E:143:LYS:HD3	1:E:149:GLU:O	2.13	0.47
1:A:66:ILE:HD11	1:A:105:LEU:HB3	1.96	0.47
1:E:135:GLN:O	1:E:139:VAL:HG23	2.15	0.47
1:H:11:ARG:HB2	1:H:51:HIS:NE2	2.29	0.47
2:W:11:DC:H2''	2:W:12:DA:C8	2.48	0.47
1:B:93:LEU:HD13	1:B:186:PHE:CD2	2.48	0.47
1:G:66:ILE:HD11	1:G:105:LEU:HB3	1.97	0.47
1:H:54:SER:HG	1:H:57:ARG:HG2	1.80	0.47
1:D:89:ARG:HB2	1:D:190:TRP:CZ2	2.50	0.47
1:A:157:LEU:HD12	1:B:189:ARG:CZ	2.44	0.47
1:C:114:LEU:HD12	1:C:122:GLN:NE2	2.29	0.47
1:C:122:GLN:OE1	1:D:175:ARG:HG2	2.14	0.47
1:F:21:LEU:HD23	1:F:21:LEU:C	2.40	0.47
1:G:189:ARG:O	1:G:192:LEU:HB2	2.14	0.47
1:B:49:TYR:CD2	1:B:49:TYR:N	2.82	0.47
1:B:189:ARG:C	1:B:191:PRO:HD2	2.40	0.47
1:A:76:LEU:HA	1:A:79:LYS:HG2	1.97	0.47
1:B:33:THR:N	1:B:36:LYS:HE2	2.30	0.47
1:G:23:LEU:HG	1:G:32:ILE:HD11	1.95	0.47
1:D:10:ASN:O	1:D:14:GLU:HG3	2.15	0.47
1:A:67:GLU:CD	1:A:131:ARG:HH21	2.24	0.46
1:B:63:ILE:HG21	1:B:124:ARG:HE	1.80	0.46
1:C:70:LEU:HD23	1:C:132:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:ILE:HD11	1:C:131:ARG:HG2	1.97	0.46
1:C:181:ARG:HB2	1:C:184:ASP:OD2	2.15	0.46
1:D:52:PHE:HA	1:D:53:PRO:HD3	1.71	0.46
1:E:192:LEU:HD21	1:F:153:THR:HG21	1.97	0.46
1:H:54:SER:OG	1:H:57:ARG:HG2	2.15	0.46
1:B:66:ILE:HD12	1:B:128:LEU:HD11	1.96	0.46
1:C:9:ARG:NH1	1:C:10:ASN:H	2.12	0.46
1:D:62:LEU:HD23	1:D:108:ILE:HD11	1.97	0.46
1:B:73:ARG:HG2	1:B:94:LEU:CD1	2.45	0.46
1:C:62:LEU:HD12	1:C:62:LEU:HA	1.80	0.46
1:A:76:LEU:HA	1:A:79:LYS:HE3	1.98	0.46
1:E:153:THR:HG21	1:F:192:LEU:HD21	1.98	0.46
1:G:160:SER:CB	1:H:172:ARG:HH12	2.27	0.46
1:A:49:TYR:OH	2:Z:29:DA:H2''	2.15	0.46
1:G:100:GLU:HA	1:G:173:PHE:CE2	2.51	0.46
1:A:143:LYS:HD2	1:A:151:TYR:CZ	2.50	0.46
1:B:4:GLU:OE1	1:B:4:GLU:HA	2.15	0.46
1:B:74:ILE:HG13	1:B:94:LEU:HD23	1.98	0.46
1:F:52:PHE:CD2	1:F:58:MET:HG2	2.51	0.46
1:G:70:LEU:O	1:G:74:ILE:HG13	2.15	0.46
1:C:185:ASP:O	1:C:189:ARG:HG3	2.16	0.46
1:C:37:LEU:O	1:C:41:VAL:HG23	2.16	0.46
1:D:15:ILE:CD1	1:D:58:MET:HE3	2.46	0.46
1:D:43:VAL:CG1	1:D:44:SER:N	2.79	0.46
1:F:67:GLU:HG2	1:F:128:LEU:HG	1.98	0.46
1:E:138:GLN:O	1:E:142:GLU:HG3	2.16	0.45
1:B:43:VAL:HG22	1:B:44:SER:N	2.31	0.45
1:B:81:GLU:HA	1:B:81:GLU:OE1	2.16	0.45
1:B:83:ASP:O	1:B:84:THR:C	2.59	0.45
1:D:15:ILE:HD13	1:D:52:PHE:CE2	2.50	0.45
1:D:89:ARG:HB2	1:D:190:TRP:CE2	2.51	0.45
1:A:56:THR:HG23	1:A:121:LEU:HD11	1.97	0.45
1:C:151:TYR:CE1	1:C:197:LEU:HB3	2.51	0.45
1:D:19:LEU:HD22	1:D:58:MET:HE2	1.97	0.45
1:C:164:ALA:O	1:D:168:GLY:HA3	2.16	0.45
2:Z:23:DG:H2''	2:Z:24:DT:C5'	2.47	0.45
1:A:79:LYS:C	1:A:82:LYS:HZ2	2.25	0.45
1:E:190:TRP:HB3	1:E:191:PRO:HD3	1.98	0.45
1:G:64:GLU:HG3	1:G:124:ARG:NH2	2.24	0.45
1:H:9:ARG:NH2	4:H:207:HOH:O	2.45	0.45
2:Z:23:DG:H2''	2:Z:24:DT:H5'	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ALA:C	4:A:201:HOH:O	2.59	0.45
1:A:79:LYS:O	1:A:82:LYS:NZ	2.50	0.45
1:C:181:ARG:HA	1:C:182:PRO:HD3	1.85	0.45
1:D:120:ARG:HG2	1:D:120:ARG:NH1	2.26	0.45
1:D:173:PHE:HD1	1:D:180:TYR:O	2.00	0.45
1:E:168:GLY:O	1:E:172:ARG:HG3	2.17	0.45
1:H:95:LEU:HD21	1:H:132:ILE:HD13	1.99	0.45
2:R:2:DG:H2''	2:R:3:DT:H5'	1.98	0.45
1:E:91:ILE:O	1:E:94:LEU:HB3	2.17	0.45
1:F:171:SER:O	1:F:175:ARG:HB2	2.17	0.45
1:B:48:LEU:C	1:B:50:ARG:H	2.25	0.45
1:B:89:ARG:HB2	1:B:190:TRP:CZ2	2.52	0.45
1:E:101:ARG:C	1:E:103:PRO:HD3	2.42	0.45
1:A:87:ARG:NH2	4:A:202:HOH:O	2.42	0.45
2:Z:24:DT:H2''	2:Z:25:DG:N7	2.31	0.45
1:B:67:GLU:O	1:B:71:ILE:HG12	2.16	0.44
1:F:158:LEU:O	1:F:162:ILE:HG12	2.17	0.44
1:H:77:ILE:HD12	1:H:90:LEU:HB3	1.99	0.44
1:H:143:LYS:HD3	1:H:151:TYR:CZ	2.52	0.44
1:D:185:ASP:O	1:D:189:ARG:HG3	2.17	0.44
1:E:100:GLU:HB2	1:E:182:PRO:HD2	1.99	0.44
1:H:11:ARG:O	1:H:15:ILE:HG13	2.18	0.44
1:B:43:VAL:HG13	1:B:44:SER:O	2.17	0.44
1:G:73:ARG:O	1:G:77:ILE:HG13	2.17	0.44
1:H:49:TYR:HA	1:H:52:PHE:O	2.17	0.44
1:A:49:TYR:HB2	4:A:201:HOH:O	2.17	0.44
1:B:35:ALA:HB2	1:B:45:GLU:OE1	2.18	0.44
1:C:114:LEU:HD11	1:C:125:ILE:HG13	1.99	0.44
1:H:73:ARG:HB2	1:H:94:LEU:HD21	2.00	0.44
1:E:53:PRO:CG	1:E:57:ARG:HG3	2.46	0.44
1:E:164:ALA:O	1:F:168:GLY:HA3	2.18	0.44
1:F:14:GLU:HG2	1:F:14:GLU:H	1.66	0.44
1:G:176:SER:O	1:G:177:GLU:HB2	2.17	0.44
1:H:138:GLN:O	1:H:142:GLU:HG3	2.17	0.44
1:C:87:ARG:HH22	1:C:146:ARG:NH2	2.16	0.44
1:C:165:PHE:CE2	1:C:193:ILE:HD11	2.52	0.44
1:A:143:LYS:HD3	1:A:149:GLU:O	2.18	0.44
1:G:12:ARG:O	1:G:12:ARG:HG2	2.18	0.44
2:Z:28:DT:H2'	2:Z:29:DA:C8	2.53	0.44
1:B:181:ARG:HA	1:B:182:PRO:HD2	1.85	0.44
1:E:22:MET:HE2	1:E:32:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:36:LYS:NZ	4:R:101:HOH:O	2.50	0.44
3:K:373:ASP:O	3:K:374:ILE:C	2.60	0.44
1:F:57:ARG:HA	1:F:57:ARG:HD3	1.69	0.43
1:G:115:MET:HE3	1:H:112:HIS:HD2	1.80	0.43
1:C:62:LEU:O	1:C:66:ILE:HG13	2.17	0.43
1:G:9:ARG:HD2	1:G:12:ARG:H	1.82	0.43
1:H:59:PHE:O	1:H:63:ILE:HG13	2.17	0.43
1:C:123:GLY:O	1:C:127:GLN:HG3	2.18	0.43
1:D:71:ILE:HD11	1:D:131:ARG:HG2	2.00	0.43
1:E:147:GLU:CD	4:E:203:HOH:O	2.61	0.43
1:E:23:LEU:CD1	1:E:32:ILE:HG13	2.48	0.43
1:F:179:LYS:NZ	2:Z:27:DG:P	2.92	0.43
1:H:16:LEU:HD22	1:H:62:LEU:HD13	2.00	0.43
1:B:31:ARG:O	1:B:36:LYS:CE	2.66	0.43
1:B:49:TYR:N	1:B:49:TYR:HD2	2.16	0.43
1:C:70:LEU:O	1:C:74:ILE:HG13	2.19	0.43
1:E:9:ARG:C	1:E:11:ARG:N	2.72	0.43
1:H:176:SER:HB3	1:H:180:TYR:CD2	2.54	0.43
1:C:143:LYS:HD2	1:C:151:TYR:CE2	2.52	0.43
1:E:181:ARG:HA	1:E:182:PRO:HD3	1.91	0.43
1:F:126:ASN:O	1:F:130:GLU:HG2	2.19	0.43
1:G:154:ASP:OD2	1:G:156:THR:HB	2.19	0.43
1:E:189:ARG:HG2	1:F:157:LEU:HD21	2.00	0.43
1:B:144:ARG:HG3	1:B:150:GLY:HA3	2.01	0.42
1:H:31:ARG:NH1	1:H:116:PHE:HB3	2.34	0.42
1:H:70:LEU:O	1:H:74:ILE:HG13	2.19	0.42
1:C:9:ARG:HH11	1:C:10:ASN:H	1.66	0.42
1:D:170:LEU:O	1:D:173:PHE:HB3	2.18	0.42
1:H:89:ARG:HB2	1:H:190:TRP:CZ2	2.55	0.42
1:A:57:ARG:HA	1:A:57:ARG:HD3	1.82	0.42
1:D:176:SER:CB	1:D:180:TYR:HD2	2.32	0.42
1:G:87:ARG:HH22	1:G:146:ARG:NH2	2.16	0.42
1:G:164:ALA:O	1:H:168:GLY:HA3	2.18	0.42
1:D:73:ARG:HB2	1:D:94:LEU:HD21	2.00	0.42
1:F:10:ASN:O	1:F:13:GLU:HB3	2.18	0.42
1:H:38:ALA:HB2	1:H:48:LEU:HD22	2.02	0.42
1:C:31:ARG:NH1	1:C:116:PHE:O	2.42	0.42
1:C:49:TYR:HA	1:C:52:PHE:O	2.19	0.42
1:C:89:ARG:HB2	1:C:190:TRP:CZ2	2.55	0.42
1:C:184:ASP:O	1:C:185:ASP:HB2	2.19	0.42
1:F:16:LEU:HB3	1:F:62:LEU:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:PHE:O	1:A:63:ILE:HG13	2.20	0.42
1:A:153:THR:OG1	1:A:158:LEU:HD23	2.20	0.42
1:A:70:LEU:HD21	1:A:98:PHE:CD2	2.54	0.42
1:A:138:GLN:O	1:A:142:GLU:HG3	2.19	0.42
1:A:156:THR:OG1	1:A:157:LEU:N	2.52	0.42
1:E:37:LEU:O	1:E:41:VAL:HG23	2.19	0.42
1:F:11:ARG:C	1:F:13:GLU:H	2.28	0.42
1:A:189:ARG:O	1:A:192:LEU:HB2	2.19	0.42
1:B:72:THR:O	1:B:76:LEU:HD13	2.20	0.42
1:C:71:ILE:HG21	1:C:131:ARG:HH21	1.84	0.42
1:D:53:PRO:HD2	1:D:57:ARG:HG3	2.02	0.42
1:D:143:LYS:HD2	1:D:151:TYR:CE2	2.55	0.42
2:R:2:DG:H2''	2:R:3:DT:C5'	2.50	0.42
1:A:135:GLN:O	1:A:138:GLN:OE1	2.38	0.41
1:B:22:MET:SD	1:B:37:LEU:HD12	2.60	0.41
1:H:38:ALA:C	1:H:40:SER:H	2.28	0.41
1:H:49:TYR:N	1:H:49:TYR:CD2	2.88	0.41
1:A:47:ALA:O	1:A:50:ARG:HB2	2.20	0.41
1:A:129:PHE:CB	1:B:175:ARG:NH2	2.83	0.41
1:E:88:LEU:HD13	1:E:139:VAL:HG11	2.02	0.41
1:C:66:ILE:HD11	1:C:105:LEU:HB3	2.03	0.41
1:E:62:LEU:HD12	1:E:62:LEU:HA	1.90	0.41
1:G:73:ARG:HH21	1:G:101:ARG:CZ	2.30	0.41
1:H:176:SER:CB	1:H:180:TYR:CD2	3.04	0.41
1:B:31:ARG:O	1:B:36:LYS:HE3	2.20	0.41
1:E:57:ARG:HD3	1:E:57:ARG:HA	1.88	0.41
1:G:9:ARG:HD2	1:G:11:ARG:H	1.85	0.41
1:G:114:LEU:HB3	4:G:216:HOH:O	2.19	0.41
1:B:144:ARG:HG3	1:B:150:GLY:CA	2.49	0.41
1:H:165:PHE:CE2	1:H:193:ILE:HD11	2.55	0.41
2:T:28:DT:H2''	2:T:29:DA:C8	2.55	0.41
1:B:146:ARG:C	1:B:147:GLU:HG2	2.46	0.41
1:D:15:ILE:CG1	1:D:16:LEU:N	2.83	0.41
1:H:62:LEU:O	1:H:66:ILE:HG13	2.20	0.41
1:H:91:ILE:HG21	1:H:136:LEU:CD1	2.43	0.41
1:G:64:GLU:CG	1:G:124:ARG:HH22	2.23	0.41
1:B:85:THR:HG22	1:B:86:ALA:N	2.36	0.41
1:B:192:LEU:HD12	1:B:192:LEU:N	2.35	0.41
1:D:23:LEU:HD12	1:D:23:LEU:HA	1.79	0.41
1:E:9:ARG:HG3	1:E:10:ASN:N	2.35	0.41
1:E:161:GLN:HE22	1:F:193:ILE:HD11	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:190:TRP:HB3	1:H:191:PRO:HD3	2.03	0.41
1:E:47:ALA:HB2	2:T:24:DT:OP2	2.21	0.41
1:E:82:LYS:HA	1:E:82:LYS:HD3	1.89	0.41
1:H:34:THR:HG21	1:H:49:TYR:OH	2.21	0.41
1:H:163:LEU:HD23	1:H:163:LEU:HA	1.83	0.41
1:B:16:LEU:N	1:B:16:LEU:HD12	2.36	0.40
1:B:158:LEU:HD21	1:B:196:GLN:O	2.21	0.40
1:C:57:ARG:HA	1:C:60:ASP:HB2	2.01	0.40
1:E:130:GLU:O	4:E:201:HOH:O	2.21	0.40
1:F:73:ARG:HB3	3:K:372:LEU:CD2	2.52	0.40
1:H:23:LEU:HD13	1:H:32:ILE:CD1	2.49	0.40
1:A:89:ARG:HB2	1:A:190:TRP:CE2	2.56	0.40
1:A:190:TRP:HB3	1:A:191:PRO:HD3	2.04	0.40
1:E:144:ARG:NH1	1:E:150:GLY:HA3	2.36	0.40
1:G:143:LYS:HD2	1:G:151:TYR:CZ	2.56	0.40
1:H:83:ASP:HB3	1:H:86:ALA:HB3	2.02	0.40
1:B:38:ALA:HB1	1:B:43:VAL:O	2.21	0.40
1:E:9:ARG:HD2	1:E:10:ASN:OD1	2.21	0.40
1:B:189:ARG:HA	1:B:192:LEU:HD13	2.03	0.40
1:E:11:ARG:HG3	1:E:12:ARG:H	1.87	0.40
1:G:142:GLU:HG2	1:G:146:ARG:NE	2.30	0.40
1:A:123:GLY:O	1:A:127:GLN:HG3	2.21	0.40
1:B:142:GLU:HB3	1:B:146:ARG:HE	1.85	0.40
1:D:34:THR:HG21	1:D:49:TYR:OH	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	188/196 (96%)	176 (94%)	11 (6%)	1 (0%)	24 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	194/196 (99%)	171 (88%)	21 (11%)	2 (1%)	12	28
1	C	188/196 (96%)	181 (96%)	7 (4%)	0	100	100
1	D	187/196 (95%)	184 (98%)	3 (2%)	0	100	100
1	E	188/196 (96%)	180 (96%)	7 (4%)	1 (0%)	24	46
1	F	187/196 (95%)	185 (99%)	2 (1%)	0	100	100
1	G	188/196 (96%)	181 (96%)	7 (4%)	0	100	100
1	H	188/196 (96%)	181 (96%)	7 (4%)	0	100	100
3	K	6/10 (60%)	5 (83%)	1 (17%)	0	100	100
All	All	1514/1578 (96%)	1444 (95%)	66 (4%)	4 (0%)	36	58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	12	ARG
1	E	10	ASN
1	A	53	PRO
1	B	84	THR

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	166/170 (98%)	158 (95%)	8 (5%)	23	47
1	B	170/170 (100%)	159 (94%)	11 (6%)	15	35
1	C	166/170 (98%)	157 (95%)	9 (5%)	20	42
1	D	165/170 (97%)	151 (92%)	14 (8%)	10	22
1	E	166/170 (98%)	153 (92%)	13 (8%)	11	26
1	F	165/170 (97%)	152 (92%)	13 (8%)	11	26
1	G	166/170 (98%)	153 (92%)	13 (8%)	11	26
1	H	166/170 (98%)	152 (92%)	14 (8%)	10	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	K	7/9 (78%)	6 (86%)	1 (14%)	3	6
All	All	1337/1369 (98%)	1241 (93%)	96 (7%)	13	30

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLU
1	A	62	LEU
1	A	71	ILE
1	A	136	LEU
1	A	138	GLN
1	A	140	LEU
1	A	153	THR
1	A	177	GLU
1	B	18	SER
1	B	19	LEU
1	B	21	LEU
1	B	54	SER
1	B	73	ARG
1	B	85	THR
1	B	117	GLU
1	B	128	LEU
1	B	147	GLU
1	B	175	ARG
1	B	184	ASP
1	C	13	GLU
1	C	19	LEU
1	C	26	SER
1	C	62	LEU
1	C	67	GLU
1	C	70	LEU
1	C	88	LEU
1	C	96	LEU
1	C	130	GLU
1	D	18	SER
1	D	23	LEU
1	D	33	THR
1	D	36	LYS
1	D	48	LEU
1	D	50	ARG
1	D	117	GLU
1	D	128	LEU

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Mol	Chain	Res	Type
1	D	131	ARG
1	D	136	LEU
1	D	140	LEU
1	D	141	ARG
1	D	145	MET
1	D	163	LEU
1	E	11	ARG
1	E	15	ILE
1	E	48	LEU
1	E	62	LEU
1	E	87	ARG
1	E	88	LEU
1	E	94	LEU
1	E	96	LEU
1	E	122	GLN
1	E	126	ASN
1	E	131	ARG
1	E	140	LEU
1	E	192	LEU
1	F	11	ARG
1	F	12	ARG
1	F	30	GLN
1	F	57	ARG
1	F	70	LEU
1	F	96	LEU
1	F	128	LEU
1	F	136	LEU
1	F	137	ARG
1	F	145	MET
1	F	158	LEU
1	F	179	LYS
1	F	192	LEU
1	G	9	ARG
1	G	17	GLN
1	G	19	LEU
1	G	24	GLU
1	G	48	LEU
1	G	62	LEU
1	G	73	ARG
1	G	88	LEU
1	G	130	GLU
1	G	131	ARG

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Mol	Chain	Res	Type
1	G	179	LYS
1	G	187	ASP
1	G	192	LEU
1	H	23	LEU
1	H	36	LYS
1	H	40	SER
1	H	48	LEU
1	H	87	ARG
1	H	118	GLN
1	H	124	ARG
1	H	128	LEU
1	H	137	ARG
1	H	152	THR
1	H	153	THR
1	H	163	LEU
1	H	175	ARG
1	H	192	LEU
3	K	374	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	B	127	GLN
1	B	135	GLN
1	B	198	GLN
1	C	10	ASN
1	C	51	HIS
1	D	118	GLN
1	D	122	GLN
1	D	127	GLN
1	E	122	GLN
1	E	126	ASN
1	F	30	GLN
1	F	122	GLN
1	F	126	ASN
1	G	51	HIS
1	G	118	GLN
1	G	122	GLN
1	H	135	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	190/196 (96%)	0.93	26 (13%) 6 5	27, 67, 132, 150	0
1	B	196/196 (100%)	1.11	30 (15%) 5 4	32, 73, 115, 192	0
1	C	190/196 (96%)	-0.02	4 (2%) 63 58	13, 36, 70, 138	0
1	D	189/196 (96%)	0.15	8 (4%) 40 35	12, 36, 86, 104	0
1	E	190/196 (96%)	0.21	8 (4%) 40 35	25, 46, 87, 127	0
1	F	189/196 (96%)	0.34	3 (1%) 70 66	27, 49, 95, 116	0
1	G	190/196 (96%)	0.14	8 (4%) 40 35	20, 41, 79, 110	0
1	H	190/196 (96%)	0.26	5 (2%) 57 51	21, 43, 85, 118	0
2	R	12/12 (100%)	0.10	0 100 100	43, 59, 84, 88	0
2	T	12/12 (100%)	-0.05	0 100 100	41, 54, 80, 82	0
2	W	12/12 (100%)	0.41	0 100 100	35, 55, 89, 94	0
2	Z	12/12 (100%)	0.27	0 100 100	48, 58, 83, 84	0
3	K	8/10 (80%)	2.60	5 (62%) 0 0	82, 117, 127, 132	0
All	All	1580/1626 (97%)	0.40	97 (6%) 27 22	12, 49, 102, 192	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	ALA	5.9
1	A	76	LEU	5.3
1	A	153	THR	4.9
1	H	148	GLY	4.6
3	K	372	LEU	4.3
3	K	375	PRO	3.8
1	A	145	MET	3.7
1	A	140	LEU	3.7
1	H	149	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	151	TYR	3.5
1	B	8	LYS	3.4
1	A	138	GLN	3.4
1	A	141	ARG	3.2
1	E	181	ARG	3.2
1	A	150	GLY	3.2
1	B	46	ALA	3.1
3	K	374	ILE	3.1
1	B	180	TYR	3.1
1	B	5	LYS	3.1
1	A	157	LEU	3.0
1	E	9	ARG	3.0
1	G	9	ARG	3.0
1	D	149	GLU	2.9
1	A	24	GLU	2.9
1	C	9	ARG	2.9
1	G	28	GLY	2.9
1	B	7	ALA	2.9
1	A	77	ILE	2.8
1	A	152	THR	2.8
1	H	144	ARG	2.8
1	A	158	LEU	2.8
1	A	84	THR	2.8
1	D	50	ARG	2.8
1	D	141	ARG	2.8
1	G	10	ASN	2.7
1	B	148	GLY	2.7
1	B	4	GLU	2.7
1	B	95	LEU	2.6
1	G	144	ARG	2.6
1	B	47	ALA	2.6
1	A	139	VAL	2.6
1	B	191	PRO	2.6
1	F	47	ALA	2.6
1	B	51	HIS	2.5
3	K	377	PHE	2.5
1	G	180	TYR	2.5
1	A	148	GLY	2.5
1	D	43	VAL	2.5
1	A	136	LEU	2.5
1	B	144	ARG	2.5
1	B	190	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	12	ARG	2.4
1	A	142	GLU	2.4
1	H	11	ARG	2.4
1	B	36	LYS	2.4
1	D	55	LYS	2.4
1	B	186	PHE	2.4
1	F	149	GLU	2.4
1	D	47	ALA	2.4
1	E	145	MET	2.4
1	A	73	ARG	2.4
1	B	59	PHE	2.4
1	E	180	TYR	2.3
1	F	51	HIS	2.3
1	A	31	ARG	2.3
1	C	10	ASN	2.3
1	A	79	LYS	2.2
1	E	11	ARG	2.2
1	G	12	ARG	2.2
1	B	6	GLN	2.2
1	A	50	ARG	2.2
1	E	146	ARG	2.2
1	B	42	GLY	2.2
1	B	187	ASP	2.2
1	A	197	LEU	2.2
1	B	53	PRO	2.2
3	K	378	LEU	2.2
1	C	12	ARG	2.2
1	A	101	ARG	2.1
1	B	23	LEU	2.1
1	B	115	MET	2.1
1	A	78	LEU	2.1
1	B	105	LEU	2.1
1	B	183	THR	2.1
1	B	145	MET	2.1
1	A	52	PHE	2.1
1	B	98	PHE	2.1
1	B	181	ARG	2.1
1	C	11	ARG	2.1
1	D	21	LEU	2.1
1	H	46	ALA	2.0
1	G	118	GLN	2.0
1	B	99	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	57	ARG	2.0
1	D	118	GLN	2.0
1	G	30	GLN	2.0
1	E	144	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.