



# Full wwPDB X-ray Structure Validation Report ⓘ

May 20, 2025 – 12:05 AM EDT

PDB ID : 3FZJ / pdb\_00003fzj  
Title : TsaR low resolution crystal structure, tetragonal form  
Authors : Monferrer, D.; Tralau, T.; Kertesz, M.A.; Dix, I.; Kikhney, A.G.; Svergun, D.I.; Uson, I.  
Deposited on : 2009-01-26  
Resolution : 7.10 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

<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>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

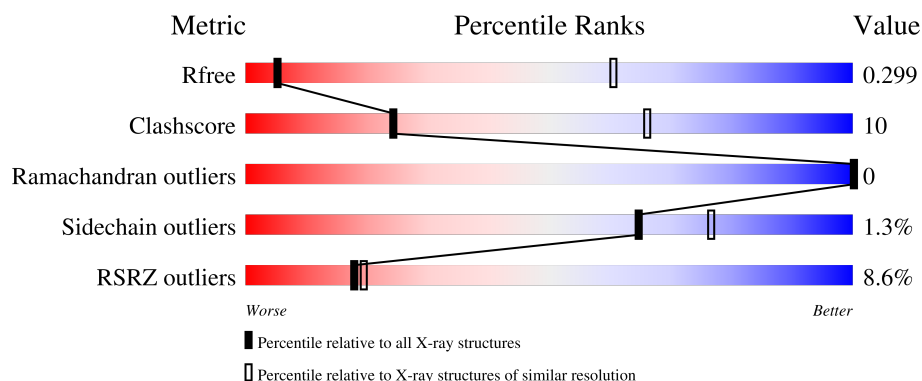
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 7.10 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))
$R_{free}$	164625	1107 (10.00-4.00)
Clashscore	180529	1146 (10.00-4.00)
Ramachandran outliers	177936	1014 (10.00-4.00)
Sidechain outliers	177891	1035 (10.00-3.96)
RSRZ outliers	164620	1102 (10.00-4.00)

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  $\geq 3$ , 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	305	<div> <div>8%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>
1	B	305	<div> <div>7%</div> <div>85%</div> <div>11%</div> <div>.</div> </div>
1	C	305	<div> <div>6%</div> <div>85%</div> <div>12%</div> <div>.</div> </div>
1	D	305	<div> <div>8%</div> <div>87%</div> <div>10%</div> <div>..</div> </div>
1	E	305	<div> <div>9%</div> <div>83%</div> <div>13%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	305	<div><div></div><div>8%</div><div>87%</div><div>9%</div><div></div></div>
1	G	305	<div><div></div><div>10%</div><div>86%</div><div>11%</div><div></div></div>
1	H	305	<div><div></div><div>7%</div><div>85%</div><div>12%</div><div></div></div>
1	I	305	<div><div></div><div>12%</div><div>84%</div><div>13%</div><div></div></div>
1	J	305	<div><div></div><div>10%</div><div>86%</div><div>11%</div><div></div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 22575 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 LysR type regulator of tsaMBCD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	1	0
			2277	1450	409	409	9			
1	B	296	Total	C	N	O	S	0	2	0
			2238	1420	403	406	9			
1	C	296	Total	C	N	O	S	0	1	0
			2277	1450	409	409	9			
1	D	296	Total	C	N	O	S	0	2	0
			2238	1420	403	406	9			
1	E	296	Total	C	N	O	S	0	1	0
			2277	1450	409	409	9			
1	F	296	Total	C	N	O	S	0	2	0
			2238	1420	403	406	9			
1	G	296	Total	C	N	O	S	0	1	0
			2277	1450	409	409	9			
1	H	296	Total	C	N	O	S	0	2	0
			2238	1420	403	406	9			
1	I	296	Total	C	N	O	S	0	1	0
			2277	1450	409	409	9			
1	J	296	Total	C	N	O	S	0	2	0
			2238	1420	403	406	9			

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	LEU	-	SEE REMARK 999	UNP P94678
A	300	HIS	-	expression tag	UNP P94678
A	301	HIS	-	expression tag	UNP P94678
A	302	HIS	-	expression tag	UNP P94678
A	303	HIS	-	expression tag	UNP P94678
A	304	HIS	-	expression tag	UNP P94678
A	305	HIS	-	expression tag	UNP P94678
B	2	LEU	-	SEE REMARK 999	UNP P94678
B	300	HIS	-	expression tag	UNP P94678

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Chain	Residue	Modelled	Actual	Comment	Reference
B	301	HIS	-	expression tag	UNP P94678
B	302	HIS	-	expression tag	UNP P94678
B	303	HIS	-	expression tag	UNP P94678
B	304	HIS	-	expression tag	UNP P94678
B	305	HIS	-	expression tag	UNP P94678
C	2	LEU	-	SEE REMARK 999	UNP P94678
C	300	HIS	-	expression tag	UNP P94678
C	301	HIS	-	expression tag	UNP P94678
C	302	HIS	-	expression tag	UNP P94678
C	303	HIS	-	expression tag	UNP P94678
C	304	HIS	-	expression tag	UNP P94678
C	305	HIS	-	expression tag	UNP P94678
D	2	LEU	-	SEE REMARK 999	UNP P94678
D	300	HIS	-	expression tag	UNP P94678
D	301	HIS	-	expression tag	UNP P94678
D	302	HIS	-	expression tag	UNP P94678
D	303	HIS	-	expression tag	UNP P94678
D	304	HIS	-	expression tag	UNP P94678
D	305	HIS	-	expression tag	UNP P94678
E	2	LEU	-	SEE REMARK 999	UNP P94678
E	300	HIS	-	expression tag	UNP P94678
E	301	HIS	-	expression tag	UNP P94678
E	302	HIS	-	expression tag	UNP P94678
E	303	HIS	-	expression tag	UNP P94678
E	304	HIS	-	expression tag	UNP P94678
E	305	HIS	-	expression tag	UNP P94678
F	2	LEU	-	SEE REMARK 999	UNP P94678
F	300	HIS	-	expression tag	UNP P94678
F	301	HIS	-	expression tag	UNP P94678
F	302	HIS	-	expression tag	UNP P94678
F	303	HIS	-	expression tag	UNP P94678
F	304	HIS	-	expression tag	UNP P94678
F	305	HIS	-	expression tag	UNP P94678
G	2	LEU	-	SEE REMARK 999	UNP P94678
G	300	HIS	-	expression tag	UNP P94678
G	301	HIS	-	expression tag	UNP P94678
G	302	HIS	-	expression tag	UNP P94678
G	303	HIS	-	expression tag	UNP P94678
G	304	HIS	-	expression tag	UNP P94678
G	305	HIS	-	expression tag	UNP P94678
H	2	LEU	-	SEE REMARK 999	UNP P94678
H	300	HIS	-	expression tag	UNP P94678

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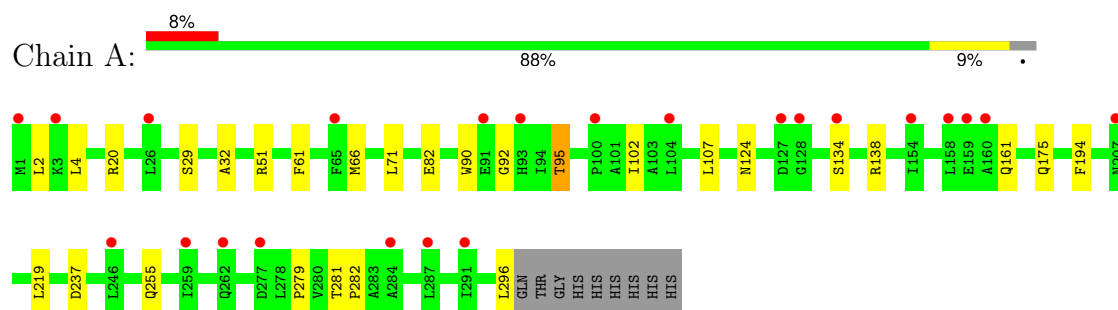
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Chain	Residue	Modelled	Actual	Comment	Reference
H	301	HIS	-	expression tag	UNP P94678
H	302	HIS	-	expression tag	UNP P94678
H	303	HIS	-	expression tag	UNP P94678
H	304	HIS	-	expression tag	UNP P94678
H	305	HIS	-	expression tag	UNP P94678
I	2	LEU	-	SEE REMARK 999	UNP P94678
I	300	HIS	-	expression tag	UNP P94678
I	301	HIS	-	expression tag	UNP P94678
I	302	HIS	-	expression tag	UNP P94678
I	303	HIS	-	expression tag	UNP P94678
I	304	HIS	-	expression tag	UNP P94678
I	305	HIS	-	expression tag	UNP P94678
J	2	LEU	-	SEE REMARK 999	UNP P94678
J	300	HIS	-	expression tag	UNP P94678
J	301	HIS	-	expression tag	UNP P94678
J	302	HIS	-	expression tag	UNP P94678
J	303	HIS	-	expression tag	UNP P94678
J	304	HIS	-	expression tag	UNP P94678
J	305	HIS	-	expression tag	UNP P94678

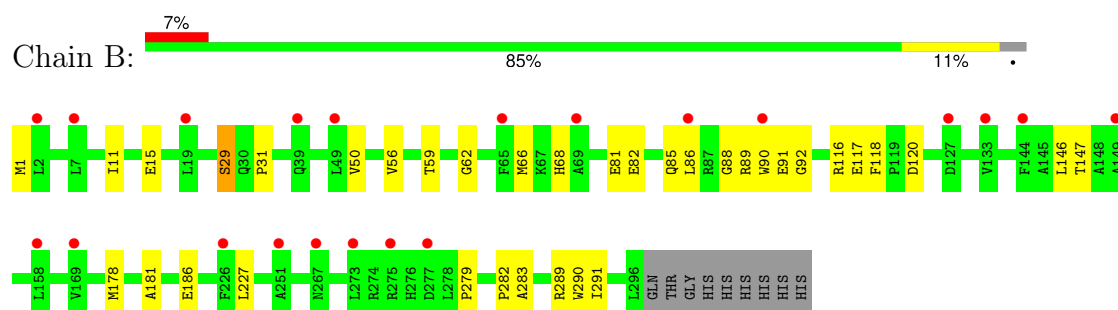
### 3 Residue-property plots [i](#)

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

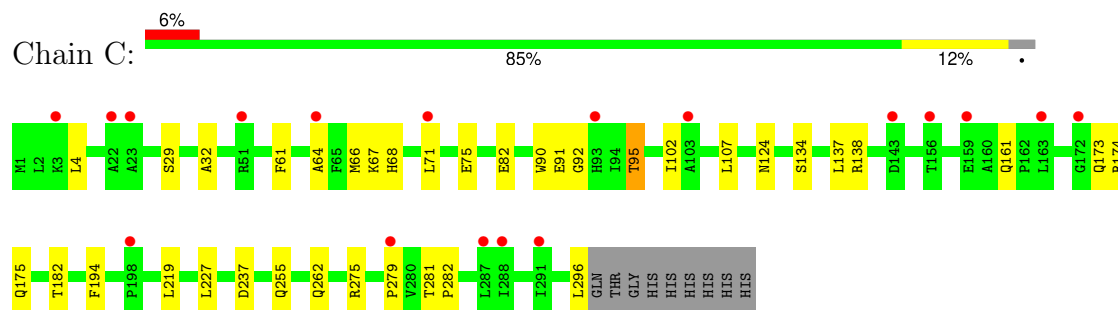
- Molecule 1: LysR type regulator of tsaMBCD



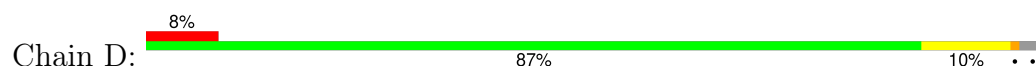
- Molecule 1: LysR type regulator of tsaMBCD



- Molecule 1: LysR type regulator of tsaMBCD



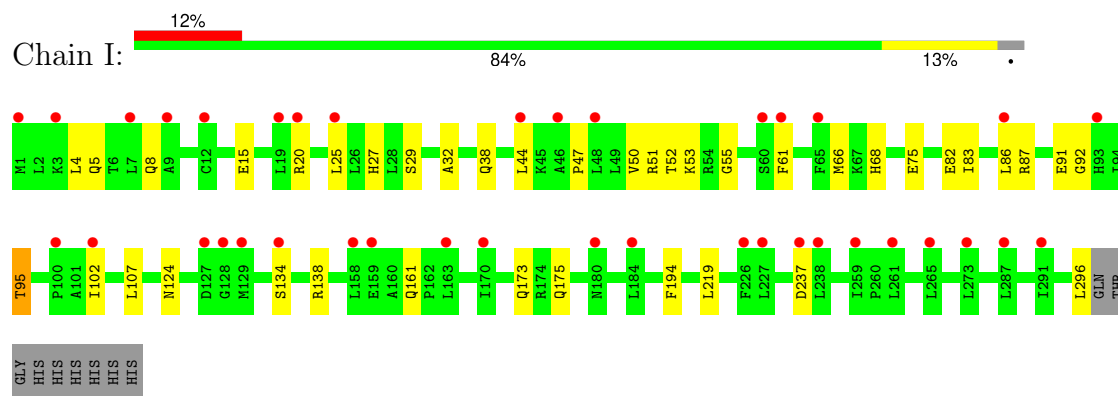
- Molecule 1: LysR type regulator of tsaMBCD



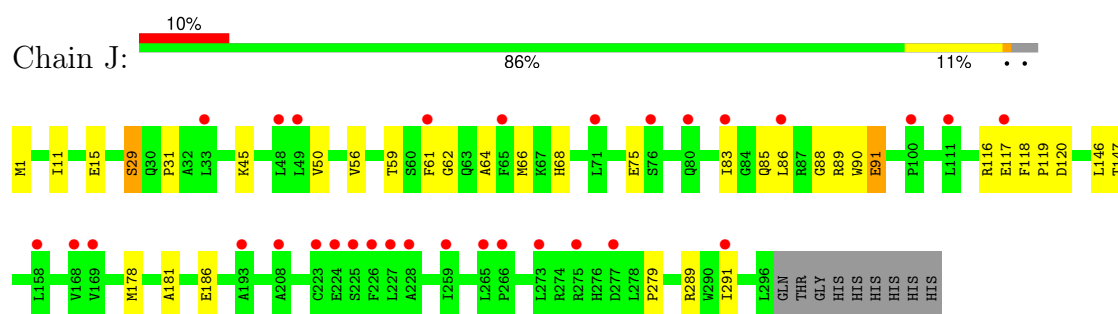




• Molecule 1: LysR type regulator of tsaMBCD



• Molecule 1: LysR type regulator of tsaMBCD



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	204.37 Å   204.37 Å   336.21 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	42.34 – 7.10 42.34 – 7.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (42.34-7.10) 99.2 (42.34-7.10)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program		Depositor
R, $R_{free}$	(Not available) , (Not available) 0.305 , 0.299	Depositor DCC
$R_{free}$ test set	535 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 173.4	EDS
L-test for twinning <sup>1</sup>	$\langle  L  \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.71	EDS
Total number of atoms	22575	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

<sup>1</sup>Theoretical 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

### 5.1 Standard geometry

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	0.74	0/2326	0.83	0/3168
1	B	0.79	0/2292	0.92	3/3122 (0.1%)
1	C	0.74	0/2326	0.82	0/3168
1	D	1.06	1/2292 (0.0%)	0.86	0/3122
1	E	0.74	0/2326	0.82	0/3168
1	F	1.13	1/2292 (0.0%)	0.94	1/3122 (0.0%)
1	G	0.74	0/2326	0.83	0/3168
1	H	0.79	0/2291	0.85	0/3119
1	I	0.74	0/2326	0.82	0/3168
1	J	0.84	1/2292 (0.0%)	1.08	3/3122 (0.1%)
All	All	0.84	3/23089 (0.0%)	0.88	7/31447 (0.0%)

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	J	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	91	GLU	C-N	38.70	1.78	1.33
1	D	91	GLU	C-N	33.99	1.85	1.32
1	J	91	GLU	C-N	-14.87	1.16	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	91	GLU	O-C-N	-29.41	88.86	123.27
1	F	91	GLU	O-C-N	-21.92	94.19	123.12
1	J	91	GLU	CA-C-N	16.03	146.63	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	91	GLU	C-N-CA	16.03	146.63	120.51
1	B	91	GLU	O-C-N	-15.98	101.04	122.94
1	B	91	GLU	CA-C-N	8.19	143.27	123.46
1	B	91	GLU	C-N-CA	8.19	143.27	123.46

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	91	GLU	Mainchain

## 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	2277	0	2308	25	31
1	B	2238	0	2234	80	0
1	C	2277	0	2308	107	1
1	D	2238	0	2235	55	20
1	E	2277	0	2305	108	3
1	F	2238	0	2235	39	17
1	G	2277	0	2308	48	33
1	H	2238	0	2235	90	0
1	I	2277	0	2306	84	23
1	J	2238	0	2235	64	0
All	All	22575	0	22709	445	64

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 10.

All (445) 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:F:91:GLU:C	1:F:92:GLY:N	1.78	1.39
1:E:20:ARG:NH2	1:I:61:PHE:CE1	1.87	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:TRP:NE1	1:C:281:THR:HG22	1.07	1.36
1:D:91:GLU:C	1:D:92:GLY:N	1.85	1.34
1:C:68:HIS:CD2	1:D:79:ALA:HA	1.65	1.31
1:E:53:LYS:O	1:J:89:ARG:HA	1.20	1.30
1:C:237:ASP:OD2	1:E:27:HIS:CE1	1.88	1.27
1:C:90:TRP:NE1	1:C:281:THR:CG2	2.01	1.24
1:C:90:TRP:O	1:C:92:GLY:N	1.71	1.23
1:B:86:LEU:O	1:I:20:ARG:HD3	1.39	1.19
1:B:88:GLY:O	1:I:52:THR:O	1.59	1.19
1:G:86:LEU:C	1:H:61:PHE:HE1	1.51	1.17
1:A:61:PHE:CE1	1:I:20:ARG:NH2	2.12	1.17
1:C:175:GLN:HB2	1:E:26:LEU:HD21	1.21	1.17
1:G:68:HIS:CE1	1:H:279:PRO:HG2	1.81	1.16
1:C:90:TRP:CZ2	1:C:281:THR:HA	1.79	1.15
1:C:68:HIS:CG	1:D:79:ALA:HB2	1.82	1.13
1:E:90:TRP:NE1	1:E:281:THR:HG22	1.62	1.13
1:C:175:GLN:CB	1:E:26:LEU:HD21	1.78	1.12
1:E:55:GLY:HA2	1:J:88:GLY:HA3	1.23	1.11
1:E:55:GLY:HA2	1:J:88:GLY:CA	1.80	1.10
1:E:53:LYS:O	1:J:89:ARG:CA	1.99	1.10
1:H:90:TRP:HB3	1:H:118:PHE:HD1	1.08	1.09
1:G:90:TRP:O	1:G:281:THR:CG2	2.02	1.08
1:C:175:GLN:HB2	1:E:26:LEU:CD2	1.82	1.08
1:C:90:TRP:CE2	1:C:281:THR:HG22	1.89	1.06
1:E:90:TRP:CE2	1:E:281:THR:HG22	1.90	1.06
1:C:68:HIS:NE2	1:D:79:ALA:HA	1.71	1.05
1:C:90:TRP:CH2	1:C:282:PRO:HD3	1.91	1.05
1:C:175:GLN:CB	1:E:26:LEU:CD2	2.35	1.04
1:B:88:GLY:CA	1:I:55:GLY:HA2	1.87	1.04
1:C:237:ASP:CG	1:E:27:HIS:CE1	2.36	1.04
1:C:68:HIS:CD2	1:D:79:ALA:CA	2.41	1.03
1:C:90:TRP:HE1	1:C:281:THR:CG2	1.65	1.02
1:E:91:GLU:C	1:E:92:GLY:N	2.17	1.02
1:B:88:GLY:HA3	1:I:55:GLY:HA2	1.04	1.01
1:H:85:GLN:OE1	1:H:283:ALA:N	1.93	1.01
1:B:178:MET:HE3	1:B:181:ALA:HB2	1.41	1.01
1:C:255:GLN:HG2	1:E:15:GLU:OE2	1.60	1.01
1:H:85:GLN:NE2	1:H:283:ALA:HB2	1.74	1.01
1:F:178:MET:HE3	1:F:181:ALA:HB2	1.41	1.01
1:A:90:TRP:NE1	1:A:281:THR:HG22	1.76	1.00
1:C:175:GLN:NE2	1:E:8:GLN:HB3	1.76	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:MET:HE3	1:D:181:ALA:HB2	1.41	1.00
1:G:86:LEU:C	1:H:61:PHE:CE1	2.39	1.00
1:H:178:MET:HE3	1:H:181:ALA:HB2	1.42	1.00
1:C:67:LYS:HD3	1:D:279:PRO:HB3	1.42	1.00
1:H:90:TRP:CE3	1:H:118:PHE:CE1	2.50	0.99
1:J:178:MET:HE3	1:J:181:ALA:HB2	1.41	0.99
1:H:90:TRP:CD2	1:H:118:PHE:HE1	1.81	0.98
1:C:67:LYS:HB3	1:D:279:PRO:HG3	1.41	0.98
1:E:20:ARG:NH2	1:I:61:PHE:HE1	1.32	0.98
1:C:68:HIS:CB	1:D:79:ALA:HB2	1.93	0.97
1:I:87:ARG:HD3	1:J:45:LYS:O	1.64	0.97
1:B:88:GLY:HA3	1:I:55:GLY:CA	1.95	0.97
1:G:90:TRP:O	1:G:281:THR:HG21	1.65	0.96
1:B:117:GLU:HA	1:I:50:VAL:HG23	1.45	0.95
1:H:90:TRP:HB3	1:H:118:PHE:CD1	2.01	0.95
1:C:90:TRP:HZ2	1:C:281:THR:HA	1.25	0.94
1:I:75:GLU:OE2	1:J:68:HIS:ND1	2.00	0.94
1:E:90:TRP:CZ2	1:E:281:THR:HA	2.04	0.92
1:C:255:GLN:HG2	1:E:15:GLU:CD	1.95	0.92
1:B:117:GLU:CA	1:I:50:VAL:HG23	2.01	0.91
1:H:82:GLU:HA	1:H:282:PRO:HD2	1.51	0.91
1:A:71:LEU:HD11	1:B:279:PRO:HD3	1.53	0.90
1:E:86:LEU:HB3	1:F:61:PHE:CE1	2.05	0.90
1:B:117:GLU:C	1:I:50:VAL:HG23	1.96	0.89
1:C:68:HIS:CG	1:D:79:ALA:CB	2.56	0.89
1:H:90:TRP:CD2	1:H:118:PHE:CE1	2.60	0.89
1:G:90:TRP:O	1:G:281:THR:HG22	1.72	0.89
1:H:85:GLN:NE2	1:H:283:ALA:CB	2.36	0.88
1:I:87:ARG:CD	1:J:45:LYS:O	2.22	0.88
1:B:86:LEU:HB3	1:I:20:ARG:NH1	1.89	0.88
1:H:91:GLU:C	1:H:92:GLY:N	2.32	0.88
1:B:89:ARG:HA	1:I:53:LYS:HA	1.54	0.87
1:C:90:TRP:CD1	1:C:281:THR:HG22	2.10	0.87
1:E:53:LYS:C	1:J:89:ARG:HA	1.99	0.87
1:C:67:LYS:CB	1:D:279:PRO:HG3	2.04	0.87
1:C:237:ASP:OD2	1:E:27:HIS:NE2	2.09	0.85
1:H:90:TRP:CB	1:H:118:PHE:HD1	1.88	0.85
1:E:86:LEU:HB3	1:F:61:PHE:HE1	1.40	0.85
1:C:90:TRP:CH2	1:C:282:PRO:CD	2.58	0.84
1:C:175:GLN:NE2	1:E:8:GLN:CB	2.40	0.84
1:A:82:GLU:OE1	1:B:68:HIS:NE2	2.12	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:GLN:HB3	1:E:26:LEU:CD2	2.09	0.83
1:J:90:TRP:O	1:J:120:ASP:HB2	1.78	0.82
1:H:90:TRP:CE3	1:H:118:PHE:HE1	1.95	0.82
1:E:55:GLY:CA	1:J:88:GLY:HA3	2.06	0.82
1:C:61:PHE:CE1	1:D:87:ARG:HG2	2.14	0.82
1:E:279:PRO:HD3	1:F:50:VAL:CG1	2.09	0.82
1:H:85:GLN:CB	1:H:282:PRO:HB2	2.09	0.81
1:C:61:PHE:HE1	1:D:87:ARG:HG2	1.44	0.81
1:I:91:GLU:C	1:I:92:GLY:N	2.38	0.81
1:C:68:HIS:CD2	1:D:79:ALA:CB	2.63	0.81
1:B:86:LEU:HB3	1:I:20:ARG:HH11	1.45	0.81
1:E:95:THR:HB	1:E:124:ASN:HB3	1.63	0.81
1:A:95:THR:HB	1:A:124:ASN:HB3	1.63	0.80
1:B:117:GLU:O	1:I:50:VAL:HG23	1.82	0.80
1:C:255:GLN:CG	1:E:15:GLU:OE2	2.30	0.80
1:G:95:THR:HB	1:G:124:ASN:HB3	1.63	0.79
1:C:175:GLN:HB3	1:E:26:LEU:HD22	1.63	0.79
1:H:91:GLU:C	1:H:121:VAL:HG22	2.07	0.79
1:E:90:TRP:NE1	1:E:281:THR:CG2	2.44	0.79
1:C:95:THR:HB	1:C:124:ASN:HB3	1.63	0.78
1:I:95:THR:HB	1:I:124:ASN:HB3	1.63	0.78
1:I:86:LEU:HB3	1:J:61:PHE:CE1	2.19	0.78
1:E:279:PRO:HD3	1:F:50:VAL:HG11	1.66	0.77
1:G:82:GLU:CD	1:H:64:ALA:HB1	2.08	0.77
1:G:86:LEU:CB	1:H:61:PHE:CD1	2.69	0.76
1:I:68:HIS:ND1	1:J:75:GLU:OE2	2.17	0.76
1:C:90:TRP:C	1:C:92:GLY:N	2.45	0.75
1:E:52:THR:O	1:J:90:TRP:HD1	1.68	0.75
1:C:90:TRP:HE1	1:C:281:THR:HG22	0.93	0.75
1:B:89:ARG:HA	1:I:53:LYS:CA	2.16	0.74
1:E:55:GLY:N	1:J:88:GLY:O	2.19	0.74
1:C:67:LYS:CD	1:D:279:PRO:HB3	2.16	0.74
1:C:75:GLU:HG2	1:D:72:ILE:HG13	1.70	0.74
1:G:86:LEU:HB3	1:H:61:PHE:CD1	2.22	0.74
1:H:85:GLN:OE1	1:H:282:PRO:HB2	1.88	0.73
1:C:75:GLU:OE2	1:D:68:HIS:HA	1.88	0.73
1:H:85:GLN:HB3	1:H:282:PRO:HB2	1.71	0.73
1:E:50:VAL:HG23	1:J:116:ARG:O	1.89	0.72
1:H:85:GLN:CD	1:H:283:ALA:H	1.97	0.72
1:G:86:LEU:HB2	1:H:61:PHE:HD1	1.53	0.71
1:B:86:LEU:O	1:I:20:ARG:CD	2.28	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:68:HIS:CE1	1:H:279:PRO:CG	2.70	0.71
1:G:87:ARG:HD3	1:H:45:LYS:O	1.90	0.71
1:G:87:ARG:CD	1:H:45:LYS:O	2.38	0.71
1:A:71:LEU:HD11	1:B:279:PRO:CD	2.20	0.70
1:C:237:ASP:CG	1:E:27:HIS:HE1	1.98	0.70
1:C:71:LEU:HD12	1:D:75:GLU:OE2	1.90	0.70
1:C:175:GLN:NE2	1:E:8:GLN:CA	2.55	0.70
1:E:20:ARG:HD3	1:J:86:LEU:O	1.92	0.70
1:G:86:LEU:HB3	1:H:61:PHE:CE1	2.26	0.70
1:E:50:VAL:CG2	1:J:116:ARG:O	2.40	0.69
1:H:70:ARG:HD3	1:H:141:THR:HG21	1.75	0.69
1:A:90:TRP:CZ2	1:A:281:THR:HA	2.28	0.68
1:C:61:PHE:CE1	1:D:87:ARG:CG	2.76	0.68
1:C:68:HIS:NE2	1:D:79:ALA:CA	2.53	0.68
1:C:68:HIS:CE1	1:D:79:ALA:N	2.61	0.68
1:E:20:ARG:HH22	1:I:61:PHE:HE1	0.83	0.68
1:F:91:GLU:O	1:F:92:GLY:N	2.25	0.68
1:G:86:LEU:O	1:H:61:PHE:HE1	1.75	0.68
1:I:86:LEU:CB	1:J:61:PHE:CE1	2.76	0.68
1:E:279:PRO:HG3	1:F:50:VAL:HG12	1.75	0.68
1:C:91:GLU:C	1:C:92:GLY:N	2.52	0.67
1:E:279:PRO:CD	1:F:50:VAL:CG1	2.72	0.67
1:E:52:THR:O	1:J:90:TRP:CD1	2.48	0.67
1:H:178:MET:CE	1:H:181:ALA:HB2	2.23	0.67
1:E:90:TRP:O	1:E:92:GLY:N	2.28	0.67
1:F:178:MET:CE	1:F:181:ALA:HB2	2.23	0.67
1:E:75:GLU:OE2	1:F:68:HIS:ND1	2.19	0.67
1:B:178:MET:CE	1:B:181:ALA:HB2	2.23	0.66
1:D:178:MET:CE	1:D:181:ALA:HB2	2.23	0.66
1:E:279:PRO:CG	1:F:50:VAL:CG1	2.74	0.66
1:I:86:LEU:C	1:J:61:PHE:HE1	2.04	0.66
1:I:44:LEU:O	1:J:83:ILE:HG21	1.96	0.66
1:I:86:LEU:CB	1:J:61:PHE:HE1	2.09	0.66
1:C:90:TRP:HH2	1:C:282:PRO:HD3	1.54	0.66
1:B:116:ARG:O	1:I:50:VAL:HG21	1.94	0.66
1:G:86:LEU:CB	1:H:61:PHE:HD1	2.09	0.66
1:G:87:ARG:N	1:H:61:PHE:CE1	2.63	0.66
1:B:90:TRP:CE3	1:B:118:PHE:CD1	2.84	0.66
1:B:86:LEU:CB	1:I:20:ARG:HH11	2.09	0.65
1:B:89:ARG:HA	1:I:53:LYS:O	1.96	0.65
1:C:175:GLN:HE22	1:E:8:GLN:CB	2.07	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289[B]:ARG:CD	1:I:38:GLN:OE1	2.44	0.65
1:A:71:LEU:CD1	1:B:279:PRO:CD	2.74	0.65
1:I:86:LEU:HB3	1:J:61:PHE:HE1	1.59	0.65
1:J:178:MET:CE	1:J:181:ALA:HB2	2.23	0.65
1:B:89:ARG:HA	1:I:53:LYS:C	2.22	0.65
1:B:82:GLU:HG3	1:B:282:PRO:CD	2.27	0.65
1:B:289[B]:ARG:HD2	1:I:38:GLN:HE22	1.61	0.65
1:C:237:ASP:CB	1:E:27:HIS:HE1	2.10	0.65
1:E:279:PRO:HD3	1:F:50:VAL:HG12	1.79	0.65
1:A:4:LEU:HB3	1:B:1:MET:SD	2.37	0.65
1:I:44:LEU:O	1:J:83:ILE:CG2	2.45	0.65
1:H:82:GLU:HG3	1:H:282:PRO:HD3	1.79	0.65
1:B:86:LEU:CB	1:I:20:ARG:NH1	2.60	0.64
1:G:86:LEU:HB2	1:H:61:PHE:CD1	2.30	0.64
1:E:279:PRO:CG	1:F:50:VAL:HG12	2.28	0.64
1:B:90:TRP:O	1:B:120:ASP:HB2	1.97	0.64
1:B:117:GLU:O	1:I:50:VAL:CG2	2.45	0.64
1:C:175:GLN:HE22	1:E:8:GLN:CA	2.11	0.63
1:H:82:GLU:HG3	1:H:282:PRO:CD	2.28	0.63
1:E:54:ARG:C	1:J:88:GLY:O	2.42	0.63
1:E:83:ILE:HG21	1:F:44:LEU:HB3	1.81	0.63
1:E:4:LEU:HB3	1:F:1:MET:SD	2.38	0.62
1:F:108:PRO:HB3	1:G:231:GLY:O	1.98	0.62
1:G:86:LEU:CB	1:H:61:PHE:CE1	2.81	0.62
1:E:279:PRO:CD	1:F:50:VAL:HG11	2.30	0.62
1:H:81:GLU:OE2	1:H:92:GLY:HA2	2.00	0.62
1:B:289[B]:ARG:HD3	1:I:38:GLN:OE1	1.99	0.61
1:H:85:GLN:CD	1:H:283:ALA:HB2	2.23	0.61
1:B:90:TRP:NE1	1:I:51:ARG:CB	2.29	0.61
1:H:91:GLU:HG2	1:H:120:ASP:CB	2.30	0.61
1:C:255:GLN:CD	1:E:15:GLU:OE2	2.43	0.61
1:B:82:GLU:OE2	1:B:282:PRO:HD3	2.00	0.61
1:C:175:GLN:HE21	1:E:8:GLN:C	2.08	0.61
1:I:75:GLU:CD	1:J:68:HIS:HD1	2.05	0.61
1:F:112:ALA:HB2	1:G:235:HIS:O	2.01	0.61
1:E:53:LYS:HA	1:J:90:TRP:H	1.67	0.60
1:A:90:TRP:HE1	1:A:281:THR:HG22	1.66	0.60
1:C:75:GLU:HB3	1:D:72:ILE:CG1	2.32	0.59
1:B:117:GLU:HA	1:I:50:VAL:CG2	2.27	0.59
1:C:173:GLN:NE2	1:E:25:LEU:HD23	2.17	0.59
1:A:90:TRP:CH2	1:A:282:PRO:HD3	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:82:GLU:CG	1:H:282:PRO:HD3	2.33	0.59
1:C:237:ASP:CB	1:E:27:HIS:CE1	2.86	0.58
1:C:68:HIS:CG	1:D:79:ALA:CA	2.84	0.58
1:C:90:TRP:CZ2	1:C:281:THR:CA	2.72	0.58
1:C:173:GLN:HE22	1:E:26:LEU:HD23	1.68	0.58
1:C:75:GLU:CG	1:D:72:ILE:HG13	2.32	0.58
1:B:90:TRP:HB2	1:I:51:ARG:HG3	1.81	0.58
1:E:86:LEU:CB	1:F:61:PHE:CE1	2.84	0.58
1:G:82:GLU:OE2	1:H:64:ALA:HB1	2.04	0.58
1:G:86:LEU:O	1:H:61:PHE:CE1	2.54	0.58
1:H:81:GLU:CD	1:H:92:GLY:CA	2.77	0.58
1:E:51:ARG:O	1:J:119:PRO:HD2	2.03	0.57
1:C:175:GLN:HE22	1:E:8:GLN:HA	1.70	0.57
1:H:81:GLU:CD	1:H:92:GLY:HA3	2.29	0.57
1:E:38:GLN:OE1	1:J:289[B]:ARG:CD	2.53	0.57
1:B:89:ARG:CA	1:I:53:LYS:O	2.53	0.57
1:G:90:TRP:HB2	1:H:61:PHE:HZ	1.70	0.57
1:C:71:LEU:CD1	1:D:75:GLU:OE2	2.52	0.57
1:E:90:TRP:CD1	1:E:281:THR:HG22	2.37	0.57
1:A:279:PRO:HG3	1:B:50:VAL:CG1	2.35	0.56
1:G:91:GLU:HG2	1:G:282:PRO:CD	2.34	0.56
1:E:90:TRP:CH2	1:E:282:PRO:HD3	2.40	0.56
1:I:83:ILE:HD12	1:J:61:PHE:HB3	1.85	0.56
1:C:174:ARG:NH1	1:E:11:ILE:HG21	2.21	0.56
1:E:53:LYS:C	1:J:88:GLY:O	2.49	0.56
1:I:5:GLN:HG3	1:J:1:MET:HE1	1.87	0.56
1:B:90:TRP:CZ3	1:B:118:PHE:CE1	2.93	0.56
1:E:86:LEU:HB3	1:F:61:PHE:CD1	2.40	0.56
1:C:4:LEU:HB3	1:D:1:MET:SD	2.45	0.56
1:G:2:LEU:HB3	1:H:1:MET:SD	2.46	0.56
1:H:85:GLN:CD	1:H:283:ALA:N	2.61	0.56
1:H:91:GLU:HG2	1:H:120:ASP:HB3	1.88	0.56
1:E:20:ARG:CZ	1:I:61:PHE:HE1	2.12	0.55
1:A:61:PHE:CE1	1:I:20:ARG:CZ	2.88	0.55
1:C:68:HIS:CE1	1:D:78:ARG:C	2.85	0.55
1:E:53:LYS:O	1:J:88:GLY:O	2.24	0.55
1:A:71:LEU:CD1	1:B:279:PRO:HD2	2.35	0.55
1:E:51:ARG:N	1:J:117:GLU:O	2.31	0.55
1:H:85:GLN:HE22	1:H:283:ALA:HB3	1.70	0.55
1:J:90:TRP:O	1:J:120:ASP:CB	2.51	0.55
1:B:116:ARG:O	1:I:50:VAL:CG2	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:LEU:C	1:I:20:ARG:HH11	2.16	0.54
1:I:87:ARG:HD2	1:J:45:LYS:O	2.05	0.54
1:C:71:LEU:HD13	1:D:75:GLU:CD	2.32	0.54
1:H:81:GLU:OE2	1:H:92:GLY:CA	2.56	0.54
1:H:85:GLN:OE1	1:H:282:PRO:CB	2.54	0.54
1:H:85:GLN:HE22	1:H:283:ALA:CB	2.18	0.53
1:B:85:GLN:CD	1:B:283:ALA:HB2	2.33	0.53
1:E:87:ARG:HD3	1:F:45:LYS:O	2.08	0.53
1:E:134:SER:OG	1:E:138:ARG:NH1	2.42	0.53
1:I:66:MET:HE2	1:I:66:MET:HA	1.91	0.53
1:B:88:GLY:C	1:I:55:GLY:HA2	2.34	0.53
1:H:82:GLU:HA	1:H:282:PRO:CD	2.33	0.53
1:E:66:MET:HA	1:E:66:MET:HE2	1.91	0.53
1:E:279:PRO:CD	1:F:50:VAL:HG12	2.36	0.53
1:G:66:MET:HE2	1:G:66:MET:HA	1.91	0.53
1:F:235:HIS:O	1:G:112:ALA:HB2	2.09	0.52
1:A:90:TRP:CD1	1:A:281:THR:HG22	2.43	0.52
1:A:134:SER:OG	1:A:138:ARG:NH1	2.42	0.52
1:B:81:GLU:CD	1:B:92:GLY:HA2	2.35	0.52
1:B:90:TRP:CE3	1:B:118:PHE:HD1	2.26	0.52
1:B:90:TRP:CD1	1:I:51:ARG:CA	2.57	0.52
1:B:290:TRP:CZ2	1:I:47:PRO:HG3	2.44	0.52
1:B:289[B]:ARG:HD2	1:I:38:GLN:NE2	2.22	0.52
1:H:85:GLN:HB2	1:H:282:PRO:HB2	1.88	0.52
1:C:134:SER:OG	1:C:138:ARG:NH1	2.42	0.52
1:C:255:GLN:HG2	1:E:15:GLU:OE1	2.10	0.52
1:J:178:MET:HE2	1:J:186:GLU:HB3	1.92	0.52
1:I:86:LEU:C	1:J:61:PHE:CE1	2.87	0.52
1:G:134:SER:OG	1:G:138:ARG:NH1	2.42	0.52
1:I:134:SER:OG	1:I:138:ARG:NH1	2.42	0.52
1:B:89:ARG:HB2	1:I:53:LYS:O	2.10	0.52
1:D:178:MET:HE2	1:D:186:GLU:HB3	1.92	0.52
1:G:90:TRP:CB	1:H:61:PHE:HZ	2.22	0.52
1:H:178:MET:HE2	1:H:186:GLU:HB3	1.92	0.52
1:C:66:MET:HE2	1:C:66:MET:HA	1.91	0.51
1:C:90:TRP:CZ2	1:C:282:PRO:HD3	2.42	0.51
1:I:87:ARG:HD3	1:J:45:LYS:C	2.33	0.51
1:A:66:MET:HE2	1:A:66:MET:HA	1.91	0.51
1:H:82:GLU:HG3	1:H:282:PRO:CG	2.41	0.51
1:H:91:GLU:HG2	1:H:120:ASP:HB2	1.91	0.51
1:F:178:MET:HE2	1:F:186:GLU:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:90:TRP:CG	1:H:118:PHE:CD1	2.98	0.51
1:A:279:PRO:HD3	1:B:50:VAL:HG11	1.93	0.51
1:C:175:GLN:NE2	1:E:8:GLN:C	2.69	0.51
1:E:50:VAL:HG21	1:J:116:ARG:O	2.11	0.51
1:B:178:MET:HE2	1:B:186:GLU:HB3	1.92	0.50
1:C:175:GLN:NE2	1:E:8:GLN:O	2.44	0.50
1:G:91:GLU:HA	1:G:282:PRO:HD2	1.93	0.50
1:G:87:ARG:HD2	1:H:45:LYS:O	2.11	0.50
1:I:68:HIS:CE1	1:J:279:PRO:HG2	2.47	0.49
1:E:87:ARG:CD	1:F:45:LYS:HB2	2.42	0.49
1:H:91:GLU:CA	1:H:121:VAL:HG22	2.42	0.49
1:E:55:GLY:HA2	1:J:88:GLY:C	2.37	0.49
1:A:90:TRP:CE2	1:A:281:THR:HG22	2.46	0.49
1:F:62:GLY:O	1:F:66:MET:HG2	2.13	0.49
1:H:62:GLY:O	1:H:66:MET:HG2	2.13	0.49
1:C:90:TRP:CH2	1:C:282:PRO:HD2	2.43	0.49
1:C:175:GLN:CG	1:E:26:LEU:HD21	2.40	0.49
1:E:279:PRO:HG3	1:F:50:VAL:CG1	2.41	0.49
1:H:82:GLU:CA	1:H:282:PRO:HD2	2.32	0.49
1:B:29:SER:OG	1:B:31:PRO:HD2	2.13	0.48
1:D:29:SER:OG	1:D:31:PRO:HD2	2.13	0.48
1:E:51:ARG:HB3	1:J:118:PHE:HA	1.94	0.48
1:G:91:GLU:HG2	1:G:282:PRO:HD2	1.95	0.48
1:I:4:LEU:HB3	1:J:1:MET:SD	2.53	0.48
1:B:90:TRP:HD1	1:I:52:THR:N	2.11	0.48
1:J:29:SER:OG	1:J:31:PRO:HD2	2.13	0.48
1:C:90:TRP:CD1	1:C:281:THR:CG2	2.82	0.48
1:G:83:ILE:HD11	1:H:65:PHE:HB2	1.94	0.48
1:E:50:VAL:HG23	1:J:117:GLU:HA	1.95	0.48
1:I:194:PHE:CD2	1:I:219:LEU:HD13	2.49	0.48
1:B:62:GLY:O	1:B:66:MET:HG2	2.13	0.48
1:A:194:PHE:CD2	1:A:219:LEU:HD13	2.49	0.48
1:B:227:LEU:HA	1:C:227:LEU:HD13	1.96	0.48
1:H:29:SER:OG	1:H:31:PRO:HD2	2.13	0.48
1:E:194:PHE:CD2	1:E:219:LEU:HD13	2.49	0.48
1:D:62:GLY:O	1:D:66:MET:HG2	2.13	0.48
1:J:62:GLY:O	1:J:66:MET:HG2	2.13	0.48
1:B:90:TRP:NE1	1:I:51:ARG:HB2	2.20	0.47
1:E:20:ARG:NH2	1:I:61:PHE:CZ	2.72	0.47
1:C:279:PRO:HD3	1:D:50:VAL:HG11	1.95	0.47
1:E:53:LYS:HA	1:J:90:TRP:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:29:SER:OG	1:F:31:PRO:HD2	2.13	0.47
1:G:194:PHE:CD2	1:G:219:LEU:HD13	2.49	0.47
1:C:255:GLN:OE1	1:E:15:GLU:OE2	2.33	0.47
1:C:262:GLN:OE1	1:E:88:GLY:HA3	2.15	0.47
1:C:68:HIS:HB3	1:D:79:ALA:HB2	1.89	0.47
1:E:51:ARG:NH2	1:J:85:GLN:O	2.48	0.47
1:B:90:TRP:CB	1:I:51:ARG:HG3	1.89	0.47
1:B:289[B]:ARG:HD3	1:I:38:GLN:CD	2.40	0.47
1:C:194:PHE:CD2	1:C:219:LEU:HD13	2.49	0.47
1:G:87:ARG:HA	1:H:61:PHE:CZ	2.50	0.47
1:C:182:THR:HG21	1:E:87:ARG:NH2	2.29	0.47
1:E:86:LEU:CB	1:F:61:PHE:HE1	2.19	0.47
1:C:68:HIS:HE1	1:D:78:ARG:HB3	1.80	0.47
1:H:91:GLU:CG	1:H:120:ASP:HB2	2.45	0.47
1:E:53:LYS:CA	1:J:89:ARG:HA	2.45	0.46
1:E:55:GLY:O	1:J:90:TRP:CD1	2.67	0.46
1:I:86:LEU:HB2	1:J:61:PHE:CD1	2.49	0.46
1:H:178:MET:CE	1:H:186:GLU:HB3	2.46	0.46
1:J:178:MET:CE	1:J:186:GLU:HB3	2.46	0.46
1:B:178:MET:CE	1:B:186:GLU:HB3	2.46	0.46
1:C:90:TRP:CE2	1:C:281:THR:CG2	2.79	0.46
1:E:90:TRP:CZ2	1:E:281:THR:CA	2.90	0.46
1:F:178:MET:CE	1:F:186:GLU:HB3	2.46	0.46
1:G:2:LEU:HD13	1:H:1:MET:HB3	1.98	0.46
1:B:89:ARG:CB	1:I:53:LYS:O	2.64	0.46
1:C:64:ALA:HB2	1:D:86:LEU:HD11	1.98	0.46
1:G:4:LEU:HB3	1:H:1:MET:SD	2.55	0.46
1:I:86:LEU:CB	1:J:61:PHE:CD1	2.98	0.46
1:C:61:PHE:HE1	1:D:87:ARG:CG	2.17	0.46
1:C:64:ALA:HB3	1:D:83:ILE:CD1	2.46	0.46
1:B:117:GLU:O	1:I:51:ARG:N	2.47	0.46
1:C:61:PHE:O	1:D:83:ILE:HD11	2.16	0.45
1:C:61:PHE:CZ	1:D:87:ARG:HD2	2.52	0.45
1:C:90:TRP:CZ2	1:C:282:PRO:CD	2.98	0.45
1:H:81:GLU:CD	1:H:93:HIS:H	2.24	0.45
1:B:90:TRP:CG	1:I:51:ARG:HB3	2.33	0.45
1:B:82:GLU:HG3	1:B:282:PRO:CG	2.47	0.45
1:B:11:ILE:O	1:B:15:GLU:HG2	2.17	0.45
1:E:90:TRP:CH2	1:E:281:THR:HA	2.49	0.45
1:C:67:LYS:CD	1:D:279:PRO:CB	2.92	0.45
1:D:11:ILE:O	1:D:15:GLU:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:MET:CE	1:D:186:GLU:HB3	2.46	0.45
1:G:82:GLU:OE2	1:H:67:LYS:NZ	2.47	0.45
1:H:90:TRP:CE3	1:H:118:PHE:CD1	3.03	0.45
1:B:88:GLY:O	1:I:55:GLY:N	2.49	0.45
1:C:67:LYS:HB2	1:D:279:PRO:HG3	1.94	0.45
1:H:70:ARG:HD3	1:H:141:THR:CG2	2.46	0.45
1:F:50:VAL:HG13	1:F:59:THR:HG22	1.99	0.44
1:C:68:HIS:CE1	1:D:79:ALA:CA	3.00	0.44
1:D:50:VAL:HG13	1:D:59:THR:HG22	2.00	0.44
1:H:11:ILE:O	1:H:15:GLU:HG2	2.17	0.44
1:A:90:TRP:O	1:A:92:GLY:N	2.50	0.44
1:H:50:VAL:HG13	1:H:59:THR:HG22	1.99	0.44
1:I:82:GLU:CD	1:J:64:ALA:HB1	2.43	0.44
1:J:11:ILE:O	1:J:15:GLU:HG2	2.17	0.44
1:B:85:GLN:O	1:I:51:ARG:CZ	2.66	0.44
1:E:86:LEU:CB	1:F:61:PHE:CD1	3.00	0.44
1:J:50:VAL:HG13	1:J:59:THR:HG22	2.00	0.44
1:B:289[B]:ARG:CD	1:I:38:GLN:CD	2.91	0.44
1:C:67:LYS:HD3	1:D:279:PRO:CB	2.31	0.44
1:C:71:LEU:CD1	1:D:75:GLU:CD	2.91	0.44
1:F:11:ILE:O	1:F:15:GLU:HG2	2.17	0.44
1:B:117:GLU:HG3	1:I:50:VAL:HA	1.99	0.43
1:E:55:GLY:CA	1:J:88:GLY:O	2.66	0.43
1:E:277:ASP:O	1:F:50:VAL:HB	2.17	0.43
1:G:87:ARG:HD3	1:H:45:LYS:C	2.44	0.43
1:H:85:GLN:HB3	1:H:282:PRO:CB	2.43	0.43
1:H:90:TRP:CG	1:H:118:PHE:CE1	3.05	0.43
1:B:90:TRP:CH2	1:B:118:PHE:HE1	2.35	0.43
1:C:82:GLU:OE2	1:D:64:ALA:HB1	2.18	0.43
1:H:78:ARG:HG2	1:H:281:THR:HG21	1.99	0.43
1:E:53:LYS:O	1:J:89:ARG:N	2.50	0.43
1:I:29:SER:HB3	1:I:32:ALA:HB3	2.00	0.43
1:E:29:SER:HB3	1:E:32:ALA:HB3	2.00	0.43
1:B:50:VAL:HG13	1:B:59:THR:HG22	1.99	0.43
1:A:29:SER:HB3	1:A:32:ALA:HB3	2.00	0.43
1:B:89:ARG:CA	1:I:53:LYS:HA	2.37	0.43
1:C:29:SER:HB3	1:C:32:ALA:HB3	2.00	0.43
1:D:91:GLU:C	1:D:92:GLY:CA	2.83	0.43
1:E:87:ARG:CD	1:F:45:LYS:O	2.67	0.43
1:G:86:LEU:HD11	1:H:64:ALA:CB	2.49	0.43
1:G:102:ILE:HG22	1:G:107:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:PHE:HE1	1:I:20:ARG:CZ	2.31	0.42
1:F:231:GLY:O	1:G:108:PRO:HB3	2.19	0.42
1:A:102:ILE:HG22	1:A:107:LEU:HG	2.01	0.42
1:I:102:ILE:HG22	1:I:107:LEU:HG	2.01	0.42
1:H:146:LEU:HD11	1:H:291:ILE:HD13	2.02	0.42
1:G:29:SER:HB3	1:G:32:ALA:HB3	2.00	0.42
1:H:85:GLN:CD	1:H:283:ALA:CB	2.88	0.42
1:C:75:GLU:OE2	1:D:68:HIS:ND1	2.48	0.42
1:C:102:ILE:HG22	1:C:107:LEU:HG	2.01	0.42
1:F:112:ALA:CB	1:G:235:HIS:O	2.66	0.42
1:B:90:TRP:CD2	1:B:118:PHE:HD1	2.38	0.42
1:I:44:LEU:O	1:J:83:ILE:HG22	2.19	0.42
1:B:146:LEU:HD11	1:B:291:ILE:HD13	2.02	0.41
1:D:146:LEU:HD11	1:D:291:ILE:HD13	2.02	0.41
1:J:146:LEU:HD11	1:J:291:ILE:HD13	2.02	0.41
1:G:2:LEU:CB	1:H:1:MET:SD	3.08	0.41
1:H:90:TRP:CD2	1:H:118:PHE:CD1	3.07	0.41
1:E:102:ILE:HG22	1:E:107:LEU:HG	2.01	0.41
1:F:146:LEU:HD11	1:F:291:ILE:HD13	2.02	0.41
1:B:81:GLU:CD	1:B:92:GLY:CA	2.94	0.41
1:B:82:GLU:CG	1:B:282:PRO:CD	2.97	0.41
1:E:53:LYS:O	1:J:88:GLY:C	2.64	0.41
1:G:5:GLN:HG3	1:H:1:MET:HE1	2.02	0.41
1:B:227:LEU:HD13	1:C:227:LEU:HA	2.03	0.41
1:C:237:ASP:HB3	1:E:27:HIS:HE1	1.81	0.41
1:A:2:LEU:HD13	1:B:1:MET:HB3	2.02	0.40
1:C:68:HIS:HB2	1:D:79:ALA:HB2	1.89	0.40
1:C:82:GLU:CD	1:D:64:ALA:HB1	2.45	0.40
1:C:61:PHE:O	1:D:83:ILE:CD1	2.70	0.40
1:B:82:GLU:CD	1:B:282:PRO:HD3	2.46	0.40
1:H:90:TRP:CB	1:H:118:PHE:CD1	2.78	0.40
1:C:137:LEU:O	1:C:275:ARG:HD2	2.22	0.40
1:H:82:GLU:CG	1:H:282:PRO:CD	2.97	0.40

All (64) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:88:GLY:C	1:G:51:ARG:NH2[5_545]	0.17	2.03
1:F:90:TRP:CD1	1:G:51:ARG:CD[5_545]	0.34	1.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ARG:CZ	1:D:88:GLY:O[6_544]	0.48	1.72
1:A:51:ARG:CZ	1:D:88:GLY:C[6_544]	0.77	1.43
1:G:27:HIS:CE1	1:I:237:ASP:CB[3_445]	0.99	1.21
1:A:51:ARG:NE	1:D:88:GLY:O[6_544]	1.25	0.95
1:F:90:TRP:NE1	1:G:51:ARG:CD[5_545]	1.26	0.94
1:F:90:TRP:CD1	1:G:51:ARG:CG[5_545]	1.32	0.88
1:A:51:ARG:CD	1:D:90:TRP:CD1[6_544]	1.33	0.87
1:F:88:GLY:C	1:G:51:ARG:CZ[5_545]	1.33	0.87
1:A:51:ARG:NH2	1:D:88:GLY:C[6_544]	1.35	0.85
1:F:88:GLY:O	1:G:51:ARG:NH2[5_545]	1.36	0.84
1:F:88:GLY:CA	1:G:51:ARG:NH2[5_545]	1.36	0.84
1:F:86:LEU:O	1:G:20:ARG:CD[5_545]	1.37	0.83
1:A:20:ARG:NH1	1:D:87:ARG:CG[6_544]	1.39	0.81
1:F:89:ARG:N	1:G:51:ARG:NH2[5_545]	1.39	0.81
1:A:51:ARG:NH1	1:D:88:GLY:O[6_544]	1.41	0.79
1:G:27:HIS:NE2	1:I:237:ASP:CB[3_445]	1.44	0.76
1:A:255:GLN:OE1	1:I:15:GLU:OE2[6_444]	1.46	0.74
1:F:90:TRP:CG	1:G:51:ARG:CG[5_545]	1.46	0.74
1:F:88:GLY:CA	1:G:51:ARG:CZ[5_545]	1.48	0.72
1:A:51:ARG:NH1	1:D:88:GLY:C[6_544]	1.53	0.67
1:A:51:ARG:NH1	1:D:88:GLY:CA[6_544]	1.53	0.67
1:F:90:TRP:CD1	1:G:51:ARG:NE[5_545]	1.53	0.67
1:A:51:ARG:NH2	1:D:89:ARG:N[6_544]	1.55	0.65
1:A:51:ARG:NH2	1:D:88:GLY:O[6_544]	1.55	0.65
1:E:174:ARG:NH2	1:G:260:PRO:CG[4_554]	1.55	0.65
1:F:88:GLY:CA	1:G:51:ARG:NH1[5_545]	1.55	0.65
1:G:27:HIS:CE1	1:I:237:ASP:CG[3_445]	1.55	0.65
1:F:88:GLY:O	1:G:51:ARG:CZ[5_545]	1.61	0.59
1:G:27:HIS:CD2	1:I:237:ASP:OD2[3_445]	1.63	0.57
1:A:175:GLN:NE2	1:I:8:GLN:CB[6_444]	1.65	0.55
1:A:51:ARG:NE	1:D:88:GLY:C[6_544]	1.70	0.50
1:F:90:TRP:CG	1:G:51:ARG:CD[5_545]	1.70	0.50
1:E:61:PHE:CZ	1:G:20:ARG:NH2[5_545]	1.71	0.49
1:A:20:ARG:NH2	1:C:61:PHE:CZ[6_544]	1.78	0.42
1:A:51:ARG:CG	1:D:90:TRP:CB[6_544]	1.80	0.40
1:A:255:GLN:CD	1:I:15:GLU:OE2[6_444]	1.80	0.40
1:G:25:LEU:O	1:I:237:ASP:OD1[3_445]	1.81	0.39
1:G:27:HIS:NE2	1:I:237:ASP:OD2[3_445]	1.82	0.38
1:A:20:ARG:NH1	1:D:87:ARG:CD[6_544]	1.86	0.34
1:A:175:GLN:NE2	1:I:8:GLN:CA[6_444]	1.86	0.34
1:G:27:HIS:NE2	1:I:237:ASP:CG[3_445]	1.86	0.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ARG:CZ	1:D:89:ARG:N[6_544]	1.87	0.33
1:E:61:PHE:CE1	1:G:20:ARG:NH2[5_545]	1.87	0.33
1:A:51:ARG:CG	1:D:90:TRP:CD1[6_544]	1.89	0.31
1:A:237:ASP:OD2	1:I:27:HIS:CE1[6_444]	1.94	0.26
1:G:27:HIS:CG	1:I:237:ASP:OD2[3_445]	1.94	0.26
1:G:27:HIS:ND1	1:I:237:ASP:CG[3_445]	1.95	0.25
1:A:51:ARG:CG	1:D:90:TRP:CG[6_544]	1.97	0.23
1:A:237:ASP:OD1	1:I:25:LEU:O[6_444]	1.97	0.23
1:F:90:TRP:CB	1:G:51:ARG:CG[5_545]	1.99	0.21
1:A:51:ARG:CZ	1:D:88:GLY:CA[6_544]	2.02	0.18
1:A:237:ASP:OD2	1:I:27:HIS:NE2[6_444]	2.07	0.13
1:A:237:ASP:CG	1:I:27:HIS:CE1[6_444]	2.08	0.12
1:G:26:LEU:CD2	1:I:175:GLN:CB[3_445]	2.08	0.12
1:F:88:GLY:O	1:G:51:ARG:NE[5_545]	2.10	0.10
1:G:25:LEU:CD2	1:I:173:GLN:OE1[3_445]	2.11	0.09
1:A:20:ARG:NH1	1:D:87:ARG:CB[6_544]	2.12	0.08
1:G:26:LEU:CD2	1:I:175:GLN:O[3_445]	2.12	0.08
1:A:51:ARG:NH2	1:D:89:ARG:CA[6_544]	2.15	0.05
1:A:237:ASP:CB	1:I:27:HIS:CE1[6_444]	2.16	0.04
1:A:255:GLN:CG	1:I:15:GLU:OE2[6_444]	2.16	0.04
1:G:27:HIS:CE1	1:I:237:ASP:OD2[3_445]	2.19	0.01

## 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	292/305 (96%)	286 (98%)	6 (2%)	0	100	100
1	B	295/305 (97%)	290 (98%)	5 (2%)	0	100	100
1	C	292/305 (96%)	286 (98%)	6 (2%)	0	100	100
1	D	295/305 (97%)	290 (98%)	5 (2%)	0	100	100
1	E	292/305 (96%)	286 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	295/305 (97%)	290 (98%)	5 (2%)	0	100	100
1	G	292/305 (96%)	286 (98%)	6 (2%)	0	100	100
1	H	293/305 (96%)	288 (98%)	5 (2%)	0	100	100
1	I	292/305 (96%)	286 (98%)	6 (2%)	0	100	100
1	J	295/305 (97%)	290 (98%)	5 (2%)	0	100	100
All	All	2933/3050 (96%)	2878 (98%)	55 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	237/248 (96%)	234 (99%)	3 (1%)	65	77
1	B	229/248 (92%)	226 (99%)	3 (1%)	65	77
1	C	237/248 (96%)	234 (99%)	3 (1%)	65	77
1	D	229/248 (92%)	226 (99%)	3 (1%)	65	77
1	E	237/248 (96%)	234 (99%)	3 (1%)	65	77
1	F	229/248 (92%)	226 (99%)	3 (1%)	65	77
1	G	237/248 (96%)	234 (99%)	3 (1%)	65	77
1	H	229/248 (92%)	226 (99%)	3 (1%)	65	77
1	I	237/248 (96%)	234 (99%)	3 (1%)	65	77
1	J	229/248 (92%)	226 (99%)	3 (1%)	65	77
All	All	2330/2480 (94%)	2300 (99%)	30 (1%)	65	77

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	THR
1	A	161	GLN

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Mol	Chain	Res	Type
1	A	296	LEU
1	B	29	SER
1	B	56	VAL
1	B	147	THR
1	C	95	THR
1	C	161	GLN
1	C	296	LEU
1	D	29	SER
1	D	56	VAL
1	D	147	THR
1	E	95	THR
1	E	161	GLN
1	E	296	LEU
1	F	29	SER
1	F	56	VAL
1	F	147	THR
1	G	95	THR
1	G	161	GLN
1	G	296	LEU
1	H	29	SER
1	H	56	VAL
1	H	147	THR
1	I	95	THR
1	I	161	GLN
1	I	296	LEU
1	J	29	SER
1	J	56	VAL
1	J	147	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	GLN
1	A	175	GLN
1	A	292	GLN
1	B	136	GLN
1	B	262	GLN
1	B	267	ASN
1	B	294	HIS
1	C	68	HIS
1	C	161	GLN
1	C	175	GLN

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Mol	Chain	Res	Type
1	C	292	GLN
1	D	262	GLN
1	D	294	HIS
1	E	27	HIS
1	E	161	GLN
1	E	175	GLN
1	E	292	GLN
1	F	262	GLN
1	F	267	ASN
1	F	294	HIS
1	G	161	GLN
1	G	175	GLN
1	G	292	GLN
1	H	136	GLN
1	H	262	GLN
1	H	267	ASN
1	H	294	HIS
1	I	161	GLN
1	I	175	GLN
1	I	292	GLN
1	J	262	GLN
1	J	294	HIS

### 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	1
1	A	1
1	C	1
1	I	1
1	H	1
1	E	1
1	D	1
1	F	1
1	J	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	91:GLU	C	92:GLY	N	3.41
1	A	91:GLU	C	92:GLY	N	3.14
1	C	91:GLU	C	92:GLY	N	2.52
1	I	91:GLU	C	92:GLY	N	2.38
1	H	91:GLU	C	92:GLY	N	2.32
1	E	91:GLU	C	92:GLY	N	2.17
1	D	91:GLU	C	92:GLY	N	1.85
1	F	91:GLU	C	92:GLY	N	1.78
1	J	91:GLU	C	92:GLY	N	1.16

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	296/305 (97%)	0.44	23 (7%)	20	21	8, 14, 27, 35	14 (4%)
1	B	296/305 (97%)	0.45	21 (7%)	23	24	5, 14, 26, 30	9 (3%)
1	C	296/305 (97%)	0.49	18 (6%)	28	27	8, 14, 27, 35	14 (4%)
1	D	296/305 (97%)	0.42	24 (8%)	19	21	5, 14, 26, 30	9 (3%)
1	E	296/305 (97%)	0.65	28 (9%)	15	17	8, 14, 27, 35	14 (4%)
1	F	296/305 (97%)	0.49	23 (7%)	20	21	5, 14, 26, 30	9 (3%)
1	G	296/305 (97%)	0.69	29 (9%)	14	17	8, 14, 27, 35	14 (4%)
1	H	296/305 (97%)	0.52	20 (6%)	25	24	5, 14, 26, 30	9 (3%)
1	I	296/305 (97%)	0.67	38 (12%)	9	13	8, 14, 27, 35	14 (4%)
1	J	296/305 (97%)	0.67	31 (10%)	13	16	5, 14, 26, 30	9 (3%)
All	All	2960/3050 (97%)	0.55	255 (8%)	18	19	5, 14, 26, 35	115 (3%)

All (255) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	163	LEU	9.2
1	H	223	CYS	8.0
1	I	44	LEU	7.9
1	C	291	ILE	7.4
1	I	291	ILE	6.7
1	G	1	MET	6.7
1	E	107	LEU	6.3
1	H	163	LEU	6.0
1	D	277	ASP	6.0
1	I	1	MET	5.9
1	J	208	ALA	5.8
1	I	46	ALA	5.8
1	G	287	LEU	5.6

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Mol	Chain	Res	Type	RSRZ
1	I	287	LEU	5.5
1	G	291	ILE	5.4
1	E	46	ALA	5.1
1	G	235	HIS	5.0
1	G	232	VAL	5.0
1	I	25	LEU	4.9
1	F	291	ILE	4.8
1	G	65	PHE	4.8
1	A	287	LEU	4.7
1	D	291	ILE	4.7
1	J	169	VAL	4.7
1	B	226	PHE	4.7
1	D	65	PHE	4.5
1	A	1	MET	4.4
1	I	3	LYS	4.3
1	J	86	LEU	4.2
1	J	80	GLN	4.2
1	J	61	PHE	4.1
1	A	284	ALA	4.1
1	B	65	PHE	4.1
1	D	56	VAL	4.1
1	D	275	ARG	4.0
1	G	107	LEU	4.0
1	B	267	ASN	4.0
1	D	100	PRO	3.9
1	A	291	ILE	3.9
1	J	275	ARG	3.8
1	A	246	LEU	3.8
1	H	201	PRO	3.8
1	A	3	LYS	3.7
1	I	127	ASP	3.7
1	A	154	ILE	3.7
1	E	25	LEU	3.7
1	C	3	LYS	3.6
1	E	184	LEU	3.6
1	J	100	PRO	3.6
1	I	65	PHE	3.6
1	D	278	LEU	3.6
1	E	19	LEU	3.5
1	G	164	TYR	3.5
1	G	25	LEU	3.5
1	I	226	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	J	273	LEU	3.5
1	G	101	ALA	3.5
1	F	140	GLY	3.4
1	A	65	PHE	3.4
1	E	226	PHE	3.4
1	B	277	ASP	3.4
1	A	159	GLU	3.4
1	I	9	ALA	3.2
1	E	127	ASP	3.2
1	E	1	MET	3.2
1	I	86	LEU	3.2
1	G	143	ASP	3.2
1	I	184	LEU	3.2
1	G	3	LYS	3.1
1	G	9	ALA	3.1
1	G	288	ILE	3.1
1	G	127	ASP	3.1
1	A	259	ILE	3.1
1	E	227	LEU	3.1
1	J	65	PHE	3.1
1	J	76	SER	3.1
1	F	13	ILE	3.0
1	H	76	SER	3.0
1	C	287	LEU	3.0
1	E	279	PRO	3.0
1	E	44	LEU	3.0
1	E	239	LEU	3.0
1	J	83	ILE	2.9
1	F	187	LEU	2.9
1	G	234	ALA	2.9
1	B	86	LEU	2.9
1	I	227	LEU	2.9
1	C	93	HIS	2.9
1	B	7	LEU	2.9
1	G	259	ILE	2.9
1	H	143	ASP	2.9
1	J	71	LEU	2.9
1	H	204	ILE	2.9
1	D	49	LEU	2.9
1	F	71	LEU	2.9
1	A	127	ASP	2.9
1	G	184	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	I	7	LEU	2.9
1	J	33	LEU	2.9
1	B	149	ALA	2.8
1	I	134	SER	2.8
1	J	224	GLU	2.8
1	C	172	GLY	2.8
1	H	221	LEU	2.8
1	D	127	ASP	2.8
1	E	16	VAL	2.8
1	I	129[A]	MET	2.7
1	I	128	GLY	2.7
1	I	170	ILE	2.7
1	E	3	LYS	2.7
1	E	224	GLU	2.7
1	H	107	LEU	2.7
1	F	150	HIS	2.7
1	C	22	ALA	2.7
1	J	158	LEU	2.7
1	J	227	LEU	2.7
1	F	273	LEU	2.7
1	J	291	ILE	2.7
1	J	277	ASP	2.6
1	B	69	ALA	2.6
1	D	106	ALA	2.6
1	G	129[A]	MET	2.6
1	E	65	PHE	2.6
1	B	158	LEU	2.6
1	E	48	LEU	2.6
1	C	64	ALA	2.6
1	F	144	PHE	2.6
1	A	91	GLU	2.6
1	B	90	TRP	2.6
1	C	71	LEU	2.6
1	J	193	ALA	2.6
1	J	266	PRO	2.6
1	H	72	ILE	2.6
1	A	100	PRO	2.6
1	E	33	LEU	2.6
1	E	72	ILE	2.6
1	B	2	LEU	2.6
1	I	61	PHE	2.6
1	C	288	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	103	ALA	2.5
1	A	128	GLY	2.5
1	H	241	THR	2.5
1	B	127	ASP	2.5
1	H	127	ASP	2.5
1	H	16	VAL	2.5
1	J	259	ILE	2.5
1	I	12	CYS	2.5
1	H	212	TYR	2.5
1	J	48	LEU	2.5
1	J	265	LEU	2.5
1	H	193	ALA	2.5
1	D	289[A]	ARG	2.5
1	I	19	LEU	2.5
1	J	49	LEU	2.5
1	F	255	GLN	2.5
1	D	104	LEU	2.5
1	B	275	ARG	2.5
1	G	180	ASN	2.4
1	J	228	ALA	2.4
1	A	134	SER	2.4
1	D	175	GLN	2.4
1	A	160	ALA	2.4
1	C	163	LEU	2.4
1	G	270	ILE	2.4
1	G	128	GLY	2.4
1	I	100	PRO	2.4
1	D	99	SER	2.4
1	F	145	ALA	2.4
1	D	109	LEU	2.4
1	I	265	LEU	2.4
1	A	158	LEU	2.4
1	D	287	LEU	2.4
1	E	171	VAL	2.4
1	I	20	ARG	2.4
1	G	8	GLN	2.3
1	J	168	VAL	2.3
1	B	144	PHE	2.3
1	F	278	LEU	2.3
1	H	154	ILE	2.3
1	I	93	HIS	2.3
1	E	141	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	277	ASP	2.3
1	E	277	ASP	2.3
1	B	133	VAL	2.3
1	D	10	LEU	2.3
1	E	30	GLN	2.3
1	C	279	PRO	2.3
1	J	117	GLU	2.3
1	F	149	ALA	2.3
1	C	143	ASP	2.3
1	C	159	GLU	2.3
1	H	186	GLU	2.3
1	H	184	LEU	2.3
1	I	48	LEU	2.3
1	E	257	CYS	2.3
1	J	226	PHE	2.3
1	I	237	ASP	2.3
1	B	49	LEU	2.3
1	B	273	LEU	2.3
1	G	27	HIS	2.3
1	G	196	SER	2.3
1	E	208	ALA	2.3
1	A	93	HIS	2.2
1	D	180	ASN	2.2
1	D	274	ARG	2.2
1	H	182	THR	2.2
1	F	97	ALA	2.2
1	I	159	GLU	2.2
1	I	273	LEU	2.2
1	H	139	ASP	2.2
1	D	91	GLU	2.2
1	I	180	ASN	2.2
1	F	275	ARG	2.2
1	A	26	LEU	2.2
1	E	60	SER	2.2
1	F	138	ARG	2.2
1	F	174	ARG	2.2
1	F	254	ASP	2.2
1	I	102	ILE	2.1
1	I	163	LEU	2.1
1	A	104	LEU	2.1
1	F	289[A]	ARG	2.1
1	C	198	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	219	LEU	2.1
1	I	158	LEU	2.1
1	J	225	SER	2.1
1	E	278	LEU	2.1
1	F	287	LEU	2.1
1	I	238	LEU	2.1
1	G	102	ILE	2.1
1	B	19	LEU	2.1
1	G	187	LEU	2.1
1	C	23	ALA	2.1
1	A	262	GLN	2.1
1	B	39	GLN	2.1
1	F	50	VAL	2.1
1	I	259	ILE	2.1
1	D	52	THR	2.1
1	B	169	VAL	2.0
1	H	18	SER	2.0
1	I	60	SER	2.0
1	B	251	ALA	2.0
1	C	156	THR	2.0
1	D	119	PRO	2.0
1	F	47	PRO	2.0
1	G	80	GLN	2.0
1	A	207	ASN	2.0
1	D	86	LEU	2.0
1	I	261	LEU	2.0
1	J	111	LEU	2.0
1	C	51	ARG	2.0
1	J	223	CYS	2.0
1	D	273	LEU	2.0
1	F	210	ALA	2.0
1	E	243	PRO	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides 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.