



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:07 PM GMT

PDB ID : 4XS6  
Title : Salmonella typhimurium AhpC W81F mutant  
Authors : Perkins, A.; Nelson, K.; Parsonage, D.; Poole, L.; Karplus, P.A.  
Deposited on : 2015-01-21  
Resolution : 3.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

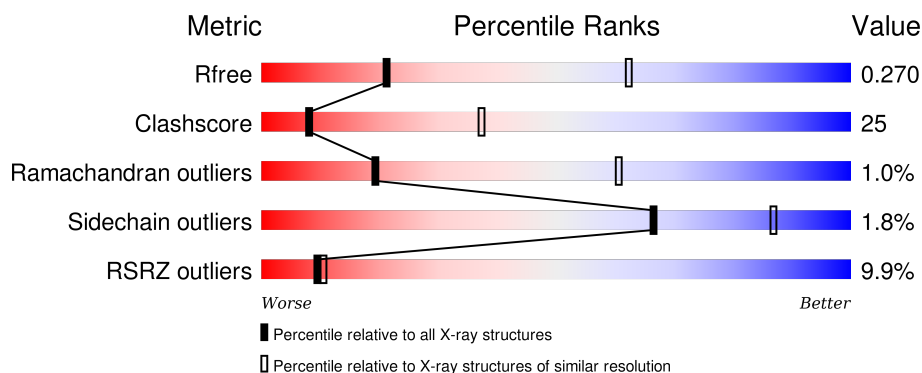
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.35 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	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)

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

Mol	Chain	Length	Quality of chain
1	A	186	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>%</span> <div style="width: 100%; height: 10px; background-color: green;"></div> <span>62%</span> <span>24%</span> <span>•</span> <span>12%</span> </div> </div>
1	B	186	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>%</span> <div style="width: 100%; height: 10px; background-color: green;"></div> <span>62%</span> <span>25%</span> <span>•</span> <span>12%</span> </div> </div>
1	C	186	<div> <div style="width: 8%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>8%</span> <div style="width: 100%; height: 10px; background-color: green;"></div> <span>70%</span> <span>17%</span> <span>13%</span> </div> </div>
1	D	186	<div> <div style="width: 9%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>9%</span> <div style="width: 100%; height: 10px; background-color: green;"></div> <span>62%</span> <span>23%</span> <span>•</span> <span>13%</span> </div> </div>
1	E	186	<div> <div style="width: 24%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>24%</span> <div style="width: 100%; height: 10px; background-color: green;"></div> <span>46%</span> <span>28%</span> <span>8%</span> <span>5%</span> <span>13%</span> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6410 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 Alkyl hydroperoxide reductase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	0	1	0
			1291	820	215	253	3			
1	B	163	Total	C	N	O	S	0	1	0
			1285	817	211	254	3			
1	C	162	Total	C	N	O	S	0	0	0
			1274	811	212	248	3			
1	D	162	Total	C	N	O	S	0	1	0
			1282	815	214	250	3			
1	E	162	Total	C	N	O	S	0	0	0
			1274	811	212	248	3			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	81	PHE	TRP	engineered mutation	UNP P0A251
B	81	PHE	TRP	engineered mutation	UNP P0A251
C	81	PHE	TRP	engineered mutation	UNP P0A251
D	81	PHE	TRP	engineered mutation	UNP P0A251
E	81	PHE	TRP	engineered mutation	UNP P0A251

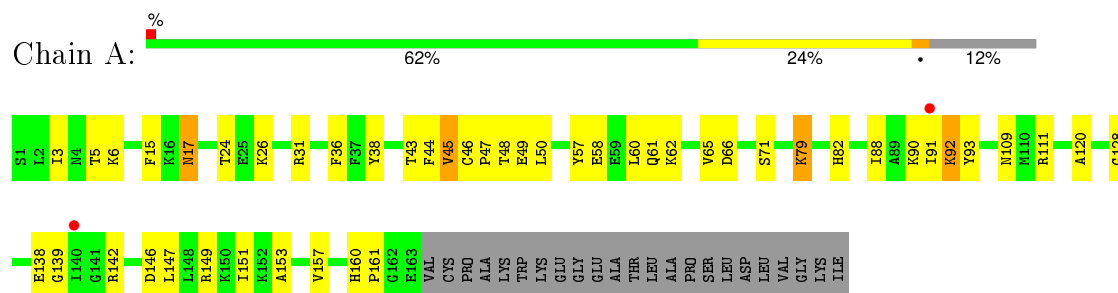
- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

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

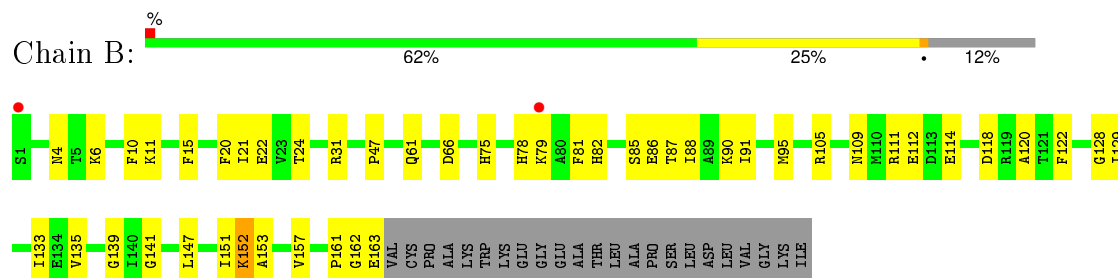
### 3 Residue-property plots

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.

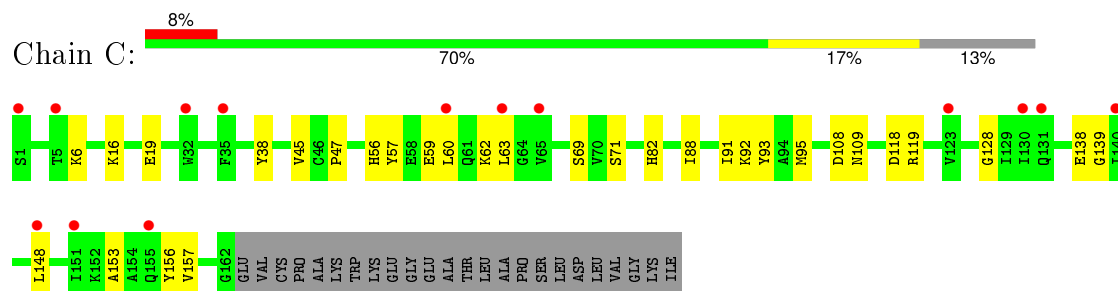
#### • Molecule 1: Alkyl hydroperoxide reductase subunit C



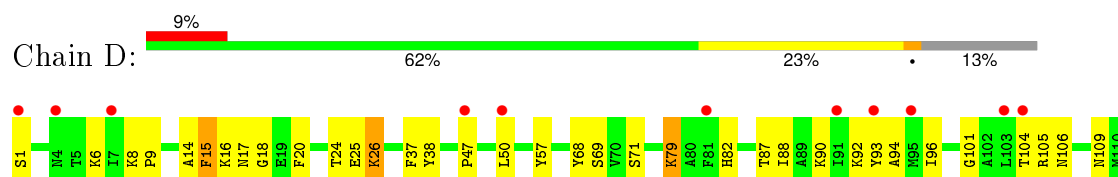
#### • Molecule 1: Alkyl hydroperoxide reductase subunit C

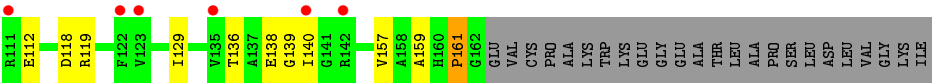


#### • Molecule 1: Alkyl hydroperoxide reductase subunit C

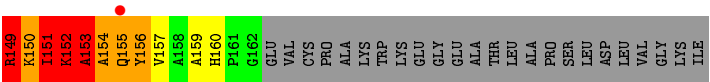
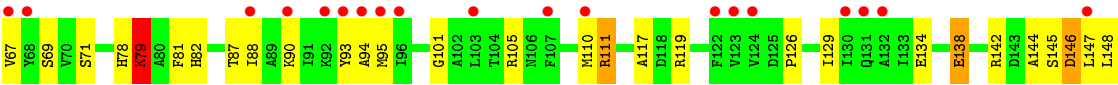
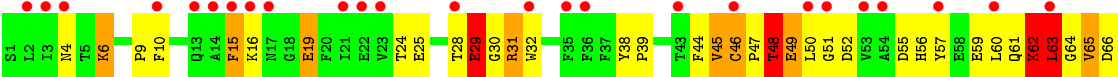


#### • Molecule 1: Alkyl hydroperoxide reductase subunit C





● Molecule 1: Alkyl hydroperoxide reductase subunit C



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.47Å 169.92Å 134.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.89 – 3.35 71.89 – 3.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (71.89-3.35) 100.0 (71.89-3.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.235 , 0.279 0.229 , 0.270	Depositor DCC
$R_{free}$ test set	1006 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	75.2	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 56.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 21099 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6410	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: K

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	0.80	0/1320	1.09	4/1787 (0.2%)
1	B	0.75	0/1314	1.03	1/1780 (0.1%)
1	C	0.72	0/1303	1.00	4/1764 (0.2%)
1	D	2.65	7/1311 (0.5%)	1.01	4/1775 (0.2%)
1	E	2.71	12/1303 (0.9%)	1.59	36/1764 (2.0%)
All	All	1.79	19/6551 (0.3%)	1.17	49/8870 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	E	0	7
All	All	0	9

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	79	LYS	CD-CE	65.43	3.14	1.51
1	D	79	LYS	CD-CE	62.85	3.08	1.51
1	D	15	PHE	CD1-CE1	33.50	2.06	1.39
1	D	15	PHE	CE1-CZ	31.46	1.97	1.37
1	E	15	PHE	CD1-CE1	30.15	1.99	1.39
1	D	15	PHE	CE2-CZ	29.98	1.94	1.37
1	E	15	PHE	CE1-CZ	29.37	1.93	1.37
1	E	15	PHE	CE2-CZ	28.26	1.91	1.37
1	D	15	PHE	CD2-CE2	27.97	1.95	1.39
1	E	15	PHE	CD2-CE2	25.62	1.90	1.39
1	E	15	PHE	CG-CD2	22.36	1.72	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	15	PHE	CG-CD1	21.53	1.71	1.38
1	E	15	PHE	CG-CD1	20.80	1.70	1.38
1	D	15	PHE	CG-CD2	19.30	1.67	1.38
1	E	153	ALA	N-CA	-6.20	1.33	1.46
1	E	65	VAL	CA-CB	5.93	1.67	1.54
1	E	150	LYS	N-CA	-5.54	1.35	1.46
1	E	46	CYS	CB-SG	5.23	1.91	1.82
1	E	48	THR	CA-CB	5.08	1.66	1.53

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	15	PHE	CB-CG-CD2	-11.29	112.89	120.80
1	E	79	LYS	CG-CD-CE	9.04	139.02	111.90
1	A	45	VAL	N-CA-C	-8.84	87.14	111.00
1	E	63	LEU	CB-CG-CD2	8.71	125.80	111.00
1	E	79	LYS	CD-CE-NZ	8.45	131.14	111.70
1	E	149	ARG	C-N-CA	-8.44	100.60	121.70
1	A	43	THR	N-CA-C	-8.41	88.29	111.00
1	E	29	GLU	C-N-CA	-7.93	105.64	122.30
1	E	63	LEU	CB-CG-CD1	-7.86	97.64	111.00
1	E	152	LYS	CA-C-N	-7.69	100.29	117.20
1	E	44	PHE	CB-CG-CD2	-7.61	115.47	120.80
1	B	162	GLY	N-CA-C	7.49	131.84	113.10
1	E	151	ILE	N-CA-C	-7.43	90.94	111.00
1	E	65	VAL	CB-CA-C	-7.28	97.57	111.40
1	E	65	VAL	N-CA-CB	7.20	127.35	111.50
1	C	156	TYR	CB-CG-CD1	7.19	125.31	121.00
1	C	156	TYR	CB-CG-CD2	-7.18	116.69	121.00
1	E	45	VAL	N-CA-C	-7.16	91.66	111.00
1	D	79	LYS	CD-CE-NZ	7.11	128.06	111.70
1	D	15	PHE	CB-CG-CD2	-7.07	115.85	120.80
1	E	62	LYS	CA-CB-CG	6.95	128.69	113.40
1	E	62	LYS	CD-CE-NZ	6.80	127.34	111.70
1	E	62	LYS	CA-C-N	-6.72	102.42	117.20
1	E	156	TYR	CA-CB-CG	6.63	126.00	113.40
1	D	79	LYS	CG-CD-CE	6.41	131.14	111.90
1	E	44	PHE	CB-CG-CD1	6.32	125.22	120.80
1	E	79	LYS	CB-CG-CD	-6.21	95.44	111.60
1	E	65	VAL	CA-CB-CG2	6.13	120.10	110.90
1	E	49	GLU	N-CA-CB	6.09	121.57	110.60
1	E	150	LYS	CD-CE-NZ	5.99	125.48	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	49	GLU	N-CA-C	-5.93	95.00	111.00
1	E	138	GLU	CA-CB-CG	5.91	126.41	113.40
1	C	60	LEU	CA-CB-CG	-5.86	101.83	115.30
1	E	111	ARG	N-CA-C	-5.84	95.24	111.00
1	E	62	LYS	C-N-CA	5.70	135.95	121.70
1	D	79	LYS	CA-CB-CG	-5.67	100.92	113.40
1	E	153	ALA	N-CA-C	-5.62	95.83	111.00
1	E	19	GLU	CA-CB-CG	-5.55	101.19	113.40
1	E	150	LYS	CA-C-N	-5.50	105.11	117.20
1	A	92	LYS	CB-CG-CD	5.47	125.83	111.60
1	E	152	LYS	CA-CB-CG	5.29	125.04	113.40
1	E	6	LYS	CA-CB-CG	5.26	124.97	113.40
1	E	46	CYS	N-CA-C	-5.21	96.92	111.00
1	E	149	ARG	N-CA-CB	5.18	119.93	110.60
1	E	63	LEU	CA-CB-CG	-5.18	103.39	115.30
1	A	92	LYS	CA-CB-CG	-5.17	102.02	113.40
1	E	31	ARG	CG-CD-NE	5.15	122.61	111.80
1	C	45	VAL	N-CA-C	-5.11	97.21	111.00
1	E	45	VAL	C-N-CA	-5.11	108.93	121.70

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	45	VAL	Peptide
1	A	62	LYS	Peptide
1	E	146	ASP	Peptide
1	E	149	ARG	Peptide
1	E	151	ILE	Peptide
1	E	154	ALA	Peptide
1	E	19	GLU	Peptide
1	E	28	THR	Peptide
1	E	29	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	1291	0	1243	39	0
1	B	1285	0	1230	37	0
1	C	1274	0	1232	25	0
1	D	1282	0	1237	72	0
1	E	1274	0	1232	144	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	D	1	0	0	0	0
All	All	6410	0	6174	310	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 25.

All (310) 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:E:15:PHE:CZ	1:E:15:PHE:CE1	1.93	1.57
1:D:15:PHE:CZ	1:D:15:PHE:CE2	1.94	1.56
1:E:15:PHE:CE2	1:E:15:PHE:CZ	1.91	1.55
1:E:15:PHE:CD2	1:E:15:PHE:CE2	1.90	1.54
1:D:15:PHE:CZ	1:D:15:PHE:CE1	1.97	1.53
1:E:15:PHE:CE1	1:E:15:PHE:CD1	1.99	1.50
1:D:15:PHE:CE2	1:D:15:PHE:CD2	1.95	1.50
1:D:15:PHE:CD1	1:D:15:PHE:CE1	2.06	1.41
1:E:29:GLU:HG2	1:E:31:ARG:HG3	1.24	1.09
1:D:15:PHE:CD1	1:D:79:LYS:CE	2.35	1.08
1:E:63:LEU:HD11	1:E:65:VAL:HG23	1.30	1.08
1:D:15:PHE:CE1	1:D:79:LYS:CD	2.36	1.08
1:E:15:PHE:CZ	1:E:79:LYS:CE	2.39	1.06
1:E:146:ASP:HB2	1:E:149:ARG:HB2	1.35	1.06
1:E:15:PHE:CD1	1:E:79:LYS:CD	2.40	1.05
1:E:15:PHE:CD2	1:E:79:LYS:CD	2.40	1.05
1:D:15:PHE:CG	1:D:79:LYS:CE	2.39	1.05
1:E:15:PHE:CE2	1:E:79:LYS:CE	2.39	1.04
1:D:15:PHE:CD2	1:D:79:LYS:CE	2.40	1.04
1:D:15:PHE:CZ	1:D:79:LYS:CD	2.42	1.02
1:D:15:PHE:CE1	1:D:79:LYS:CE	2.42	1.02
1:D:15:PHE:CE2	1:D:79:LYS:CE	2.42	1.02
1:E:15:PHE:CD1	1:E:79:LYS:HD3	1.94	1.02
1:E:15:PHE:CE1	1:E:79:LYS:CE	2.43	1.02
1:E:146:ASP:HA	1:E:149:ARG:H	1.19	1.01
1:D:15:PHE:CG	1:D:79:LYS:HE3	1.96	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:PHE:CE2	1:E:79:LYS:CD	2.44	1.01
1:E:15:PHE:CG	1:E:79:LYS:CE	2.44	1.01
1:E:15:PHE:CG	1:E:79:LYS:CD	2.44	1.00
1:E:15:PHE:CD2	1:E:79:LYS:HD2	1.96	0.99
1:E:15:PHE:CD2	1:E:79:LYS:CE	2.44	0.99
1:E:15:PHE:CE1	1:E:79:LYS:CD	2.45	0.99
1:D:15:PHE:CD1	1:D:79:LYS:CD	2.45	0.99
1:C:59:GLU:O	1:C:62:LYS:HG2	1.63	0.98
1:D:15:PHE:CZ	1:D:79:LYS:CE	2.46	0.98
1:E:15:PHE:CZ	1:E:79:LYS:HE3	1.96	0.97
1:D:15:PHE:CE2	1:D:79:LYS:CD	2.47	0.97
1:E:15:PHE:CZ	1:E:79:LYS:CD	2.49	0.96
1:B:15:PHE:HD1	1:B:79:LYS:HZ2	0.98	0.96
1:E:15:PHE:CD1	1:E:79:LYS:CE	2.48	0.96
1:D:15:PHE:CE2	1:D:79:LYS:HE2	2.02	0.95
1:C:119:ARG:HE	1:C:138:GLU:HG2	1.31	0.93
1:D:15:PHE:CD2	1:D:79:LYS:CD	2.52	0.92
1:E:29:GLU:HG2	1:E:31:ARG:CG	1.98	0.92
1:D:15:PHE:CG	1:D:79:LYS:CD	2.55	0.89
1:A:146:ASP:OD1	1:A:149:ARG:NH1	2.06	0.88
1:E:152:LYS:HB3	1:E:154:ALA:N	1.88	0.88
1:E:146:ASP:HB2	1:E:149:ARG:CB	2.03	0.87
1:E:152:LYS:HB3	1:E:154:ALA:H	1.37	0.87
1:D:15:PHE:CZ	1:D:79:LYS:HD2	2.05	0.87
1:E:63:LEU:HD11	1:E:65:VAL:CG2	2.04	0.86
1:C:59:GLU:HG3	1:C:62:LYS:HE3	1.58	0.85
1:E:29:GLU:CG	1:E:31:ARG:HG3	2.06	0.84
1:E:150:LYS:C	1:E:152:LYS:HB2	1.96	0.84
1:E:150:LYS:O	1:E:152:LYS:HB2	1.78	0.84
1:E:153:ALA:HB1	1:E:156:TYR:CB	2.07	0.84
1:E:15:PHE:CD1	1:E:79:LYS:HE2	2.14	0.83
1:E:59:GLU:O	1:E:62:LYS:HB2	1.78	0.82
1:D:15:PHE:CE2	1:D:79:LYS:HD3	2.15	0.79
1:E:16:LYS:HA	1:E:79:LYS:HZ3	1.46	0.79
1:A:46:CYS:HB3	1:A:48:THR:HG23	1.64	0.79
1:E:63:LEU:CD1	1:E:65:VAL:HG23	2.10	0.79
1:D:15:PHE:CE1	1:D:79:LYS:HD2	2.16	0.78
1:E:62:LYS:NZ	1:E:63:LEU:HB3	1.97	0.78
1:D:15:PHE:CD2	1:D:79:LYS:HE3	2.16	0.78
1:E:153:ALA:HB1	1:E:156:TYR:HB3	1.66	0.77
1:B:15:PHE:HD1	1:B:79:LYS:NZ	1.82	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:VAL:HG11	1:B:139:GLY:HA3	1.67	0.76
1:E:62:LYS:HB3	1:E:63:LEU:HD23	1.68	0.76
1:E:146:ASP:CB	1:E:149:ARG:HB2	2.13	0.75
1:E:57:TYR:CE1	1:E:93:TYR:HB3	2.22	0.75
1:C:56:HIS:HD2	1:C:148:LEU:HD12	1.51	0.74
1:B:15:PHE:CD1	1:B:79:LYS:HD3	2.23	0.74
1:E:31:ARG:NH1	1:E:66:ASP:OD1	2.20	0.73
1:E:146:ASP:HA	1:E:149:ARG:N	2.02	0.73
1:D:101:GLY:O	1:D:105:ARG:HG3	1.87	0.73
1:A:139:GLY:HA3	1:B:157:VAL:HG11	1.71	0.73
1:E:31:ARG:NH2	1:E:64:GLY:HA2	2.03	0.72
1:D:15:PHE:CD2	1:D:79:LYS:HD3	2.24	0.72
1:E:119:ARG:HE	1:E:138:GLU:HB3	1.56	0.70
1:E:101:GLY:O	1:E:105:ARG:HG2	1.91	0.70
1:B:152:LYS:HG2	1:B:153:ALA:N	2.05	0.70
1:D:15:PHE:CE1	1:D:79:LYS:NZ	2.59	0.69
1:D:17:ASN:N	1:D:79:LYS:HZ3	1.91	0.68
1:D:82:HIS:HA	1:D:88:ILE:HG22	1.75	0.68
1:B:88:ILE:HG23	1:B:91:ILE:HD12	1.74	0.68
1:D:18:GLY:N	1:D:79:LYS:NZ	2.41	0.68
1:E:63:LEU:HD13	1:E:155:GLN:HE22	1.58	0.67
1:E:148:LEU:C	1:E:150:LYS:HZ2	1.98	0.67
1:E:15:PHE:CE1	1:E:79:LYS:HE2	2.27	0.67
1:E:16:LYS:CA	1:E:79:LYS:HZ3	2.06	0.67
1:C:62:LYS:HG3	1:C:63:LEU:N	2.10	0.66
1:D:15:PHE:CD1	1:D:79:LYS:CG	2.79	0.66
1:A:15:PHE:CE1	1:A:79:LYS:HB2	2.32	0.65
1:B:20:PHE:CE1	1:B:79:LYS:HE2	2.31	0.65
1:A:6:LYS:HA	1:A:128:GLY:O	1.96	0.65
1:E:62:LYS:HZ2	1:E:63:LEU:HB3	1.60	0.65
1:E:56:HIS:O	1:E:59:GLU:HG2	1.98	0.64
1:B:109:ASN:OD1	1:B:118:ASP:HB2	1.97	0.64
1:A:17:ASN:ND2	1:A:92:LYS:HG2	2.13	0.64
1:E:150:LYS:HB3	1:E:152:LYS:HA	1.79	0.64
1:B:153:ALA:O	1:B:157:VAL:HG22	1.99	0.63
1:B:87:THR:O	1:B:90:LYS:HB2	1.98	0.63
1:C:108:ASP:O	1:D:1:SER:N	2.30	0.63
1:E:50:LEU:O	1:E:93:TYR:OH	2.16	0.63
1:D:18:GLY:N	1:D:79:LYS:HZ3	1.97	0.63
1:E:62:LYS:HD3	1:E:63:LEU:CD2	2.29	0.63
1:E:47:PRO:O	1:E:49:GLU:N	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:LYS:HA	1:C:128:GLY:O	1.98	0.62
1:D:119:ARG:HE	1:D:138:GLU:HA	1.65	0.62
1:E:32:TRP:HB3	1:E:65:VAL:HG22	1.82	0.62
1:E:47:PRO:C	1:E:49:GLU:H	2.03	0.61
1:D:15:PHE:CZ	1:D:79:LYS:HE2	2.34	0.61
1:E:152:LYS:NZ	1:E:154:ALA:HA	2.15	0.61
1:A:17:ASN:ND2	1:A:92:LYS:CG	2.64	0.61
1:D:109:ASN:OD1	1:D:118:ASP:HB2	2.01	0.61
1:E:78:HIS:HD2	1:E:95:MET:HB3	1.66	0.61
1:E:87:THR:O	1:E:90:LYS:HB2	2.01	0.60
1:D:15:PHE:HE2	1:D:82:HIS:CG	2.18	0.60
1:E:153:ALA:HB1	1:E:156:TYR:HB2	1.81	0.60
1:E:15:PHE:CD2	1:E:79:LYS:NZ	2.70	0.60
1:E:16:LYS:NZ	1:E:94:ALA:HB2	2.17	0.60
1:E:78:HIS:CD2	1:E:95:MET:HB3	2.36	0.60
1:E:15:PHE:CE2	1:E:79:LYS:HE3	2.36	0.59
1:E:156:TYR:CD1	1:E:160:HIS:HB2	2.38	0.59
1:C:59:GLU:HG3	1:C:62:LYS:CE	2.29	0.59
1:E:152:LYS:HG2	1:E:153:ALA:HB3	1.85	0.58
1:E:150:LYS:HB3	1:E:152:LYS:CA	2.33	0.58
1:B:15:PHE:HE2	1:B:82:HIS:CD2	2.21	0.58
1:A:17:ASN:HD21	1:A:92:LYS:HG2	1.68	0.58
1:E:156:TYR:O	1:E:160:HIS:N	2.36	0.57
1:A:111:ARG:HH22	1:A:138:GLU:HG3	1.68	0.57
1:A:58:GLU:HA	1:A:61:GLN:HB2	1.85	0.57
1:E:52:ASP:OD1	1:E:144:ALA:HB3	2.04	0.57
1:E:149:ARG:HG2	1:E:150:LYS:N	2.20	0.56
1:E:149:ARG:HA	1:E:150:LYS:HG2	1.86	0.56
1:B:31:ARG:NH1	1:B:66:ASP:OD1	2.38	0.56
1:E:48:THR:HA	1:E:51:GLY:H	1.71	0.56
1:E:152:LYS:HZ2	1:E:154:ALA:HA	1.71	0.56
1:A:149:ARG:NH2	1:B:141:GLY:O	2.39	0.56
1:A:31:ARG:NH1	1:A:66:ASP:OD1	2.40	0.55
1:E:15:PHE:HE2	1:E:82:HIS:CB	2.20	0.55
1:E:62:LYS:HZ2	1:E:63:LEU:CB	2.20	0.55
1:E:63:LEU:HD21	1:E:65:VAL:HG23	1.89	0.55
1:E:134:GLU:OE1	1:E:142:ARG:HG2	2.07	0.55
1:D:38:TYR:CD2	1:D:50:LEU:HD21	2.42	0.54
1:C:109:ASN:OD1	1:C:118:ASP:HB2	2.08	0.54
1:D:82:HIS:HA	1:D:88:ILE:CG2	2.37	0.54
1:B:6:LYS:HA	1:B:128:GLY:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:PRO:HA	1:D:25:GLU:HB3	1.89	0.54
1:E:10:PHE:O	1:E:24:THR:HA	2.06	0.54
1:E:144:ALA:HA	1:E:147:LEU:HB3	1.90	0.54
1:C:62:LYS:HG3	1:C:63:LEU:HG	1.90	0.54
1:D:87:THR:O	1:D:90:LYS:HG3	2.08	0.54
1:C:82:HIS:HA	1:C:88:ILE:HG22	1.90	0.53
1:B:81:PHE:O	1:B:85:SER:OG	2.25	0.53
1:E:149:ARG:CG	1:E:150:LYS:N	2.71	0.53
1:E:32:TRP:O	1:E:65:VAL:HA	2.09	0.53
1:B:31:ARG:HD3	1:B:66:ASP:OD2	2.08	0.53
1:D:8:LYS:HE2	1:D:106:ASN:OD1	2.09	0.53
1:E:61:GLN:O	1:E:64:GLY:N	2.30	0.53
1:A:157:VAL:HG11	1:B:139:GLY:CA	2.37	0.53
1:B:147:LEU:O	1:B:151:ILE:HG13	2.09	0.53
1:A:58:GLU:HG2	1:A:61:GLN:HB2	1.90	0.52
1:B:15:PHE:CD1	1:B:79:LYS:CD	2.92	0.52
1:E:105:ARG:HH21	1:E:110:MET:HG2	1.75	0.52
1:C:88:ILE:HG23	1:C:91:ILE:HD12	1.91	0.52
1:E:146:ASP:CA	1:E:149:ARG:H	2.08	0.51
1:E:32:TRP:CB	1:E:65:VAL:HG22	2.39	0.51
1:A:109:ASN:ND2	1:A:120:ALA:HB3	2.26	0.51
1:E:57:TYR:CZ	1:E:61:GLN:NE2	2.78	0.51
1:D:105:ARG:NH2	1:D:112:GLU:OE1	2.44	0.51
1:B:47:PRO:HB2	1:B:88:ILE:HD11	1.92	0.51
1:B:105:ARG:NH2	1:B:112:GLU:OE1	2.43	0.51
1:B:78:HIS:CD2	1:B:95:MET:HB3	2.46	0.51
1:C:157:VAL:HG11	1:D:139:GLY:HA3	1.93	0.51
1:C:59:GLU:HA	1:C:62:LYS:HE3	1.93	0.51
1:E:150:LYS:HB3	1:E:152:LYS:CB	2.40	0.50
1:A:38:TYR:CZ	1:A:71:SER:HB3	2.46	0.50
1:C:47:PRO:CB	1:C:88:ILE:HD11	2.42	0.50
1:A:147:LEU:O	1:A:151:ILE:HG13	2.11	0.50
1:D:105:ARG:HH21	1:D:112:GLU:CD	2.15	0.50
1:A:36:PHE:HZ	1:A:49:GLU:HB3	1.77	0.50
1:A:65:VAL:HG21	1:A:151:ILE:HG21	1.93	0.49
1:B:15:PHE:CE2	1:B:82:HIS:CG	2.99	0.49
1:C:38:TYR:CZ	1:C:71:SER:HB3	2.47	0.49
1:E:146:ASP:O	1:E:149:ARG:HB3	2.12	0.49
1:B:163:GLU:N	1:B:163:GLU:OE1	2.45	0.49
1:B:111:ARG:HD3	1:B:114:GLU:OE1	2.13	0.49
1:E:15:PHE:CE1	1:E:79:LYS:HD3	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:ALA:CB	1:E:156:TYR:HB3	2.40	0.49
1:B:10:PHE:O	1:B:24:THR:HA	2.12	0.49
1:E:39:PRO:HG3	1:E:111:ARG:NH2	2.28	0.49
1:E:119:ARG:HE	1:E:138:GLU:CB	2.24	0.49
1:A:24:THR:OG1	1:A:26:LYS:HG2	2.13	0.49
1:D:16:LYS:HB2	1:D:94:ALA:HA	1.95	0.48
1:E:63:LEU:CD2	1:E:65:VAL:HG23	2.44	0.48
1:E:31:ARG:HD3	1:E:66:ASP:OD2	2.13	0.48
1:D:16:LYS:C	1:D:79:LYS:NZ	2.67	0.48
1:D:17:ASN:CA	1:D:79:LYS:HZ3	2.26	0.48
1:E:149:ARG:HA	1:E:150:LYS:CG	2.44	0.48
1:E:55:ASP:OD1	1:E:90:LYS:HD3	2.14	0.48
1:E:47:PRO:C	1:E:49:GLU:N	2.67	0.48
1:E:156:TYR:O	1:E:159:ALA:N	2.45	0.48
1:D:18:GLY:N	1:D:79:LYS:HZ2	2.10	0.47
1:E:6:LYS:HA	1:E:129:ILE:HD13	1.96	0.47
1:E:149:ARG:HA	1:E:150:LYS:NZ	2.30	0.47
1:E:38:TYR:CZ	1:E:71:SER:HB3	2.50	0.47
1:D:79:LYS:HD3	1:D:79:LYS:HA	1.39	0.47
1:A:17:ASN:ND2	1:A:92:LYS:HG3	2.29	0.47
1:E:15:PHE:CZ	1:E:79:LYS:CG	2.96	0.47
1:E:30:GLY:HA2	1:E:126:PRO:HB3	1.97	0.47
1:E:153:ALA:O	1:E:156:TYR:HB3	2.14	0.47
1:E:59:GLU:H	1:E:59:GLU:CD	2.18	0.47
1:D:26:LYS:H	1:D:26:LYS:HG2	1.61	0.47
1:E:61:GLN:O	1:E:62:LYS:C	2.53	0.47
1:A:5:THR:HG22	1:A:6:LYS:N	2.30	0.47
1:A:50:LEU:HB3	1:A:91:ILE:HD11	1.96	0.47
1:E:150:LYS:CB	1:E:152:LYS:HA	2.44	0.46
1:A:49:GLU:OE2	1:A:142:ARG:N	2.44	0.46
1:D:15:PHE:CD1	1:D:79:LYS:NZ	2.83	0.46
1:D:17:ASN:HD21	1:D:92:LYS:HG3	1.80	0.46
1:A:82:HIS:HA	1:A:88:ILE:HG22	1.96	0.46
1:B:122:PHE:CD2	1:B:133:ILE:HG12	2.50	0.46
1:E:9:PRO:HA	1:E:25:GLU:HB3	1.98	0.46
1:A:31:ARG:HD3	1:A:66:ASP:OD2	2.15	0.46
1:C:57:TYR:HD2	1:C:92:LYS:HD3	1.79	0.46
1:E:62:LYS:HD3	1:E:63:LEU:HD22	1.98	0.46
1:E:145:SER:O	1:E:148:LEU:HB2	2.15	0.46
1:E:57:TYR:CE2	1:E:61:GLN:NE2	2.84	0.46
1:C:59:GLU:CG	1:C:62:LYS:HE3	2.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:LYS:HD3	1:E:63:LEU:HD23	1.98	0.46
1:E:156:TYR:CD1	1:E:160:HIS:CG	3.04	0.46
1:D:136:THR:HB	1:D:140:ILE:HB	1.97	0.45
1:D:17:ASN:C	1:D:79:LYS:HZ3	2.19	0.45
1:E:150:LYS:CD	1:E:152:LYS:HA	2.46	0.45
1:B:15:PHE:HE2	1:B:82:HIS:CG	2.34	0.45
1:E:156:TYR:CE1	1:E:160:HIS:HB2	2.51	0.45
1:E:39:PRO:HA	1:E:117:ALA:O	2.17	0.45
1:E:69:SER:OG	1:E:95:MET:HA	2.17	0.45
1:B:6:LYS:HA	1:B:129:ILE:HD13	1.99	0.45
1:A:3:ILE:HA	1:A:3:ILE:HD12	1.83	0.45
1:E:31:ARG:HH21	1:E:64:GLY:HA2	1.78	0.45
1:C:69:SER:OG	1:C:95:MET:HA	2.17	0.45
1:E:62:LYS:CE	1:E:63:LEU:HB3	2.46	0.44
1:C:91:ILE:HG23	1:C:93:TYR:CZ	2.52	0.44
1:C:16:LYS:O	1:C:19:GLU:HG2	2.17	0.44
1:D:57:TYR:CZ	1:D:93:TYR:HB3	2.52	0.44
1:E:62:LYS:CB	1:E:63:LEU:HD23	2.42	0.44
1:E:57:TYR:CZ	1:E:93:TYR:HB3	2.50	0.44
1:E:153:ALA:O	1:E:156:TYR:N	2.49	0.44
1:C:62:LYS:CG	1:C:63:LEU:N	2.79	0.44
1:E:45:VAL:O	1:E:47:PRO:HD3	2.17	0.44
1:D:17:ASN:HD21	1:D:92:LYS:CG	2.31	0.44
1:B:11:LYS:HZ2	1:B:22:GLU:CD	2.20	0.44
1:E:49:GLU:OE1	1:E:119:ARG:NH2	2.50	0.44
1:A:17:ASN:HD21	1:A:92:LYS:CG	2.29	0.43
1:A:58:GLU:HG2	1:A:61:GLN:HG3	1.99	0.43
1:B:11:LYS:NZ	1:B:22:GLU:OE1	2.47	0.43
1:B:20:PHE:CE1	1:B:75:HIS:HD2	2.37	0.43
1:D:6:LYS:HE2	1:D:6:LYS:HB2	1.60	0.43
1:E:88:ILE:HA	1:E:88:ILE:HD13	1.83	0.43
1:D:15:PHE:CG	1:D:79:LYS:CG	3.02	0.43
1:E:153:ALA:CA	1:E:156:TYR:H	2.31	0.43
1:E:153:ALA:HB1	1:E:156:TYR:CD2	2.53	0.43
1:E:67:VAL:O	1:E:93:TYR:HB2	2.17	0.43
1:A:15:PHE:CD1	1:A:79:LYS:HB2	2.52	0.43
1:B:21:ILE:HG22	1:B:22:GLU:N	2.34	0.43
1:D:20:PHE:CE1	1:D:79:LYS:HG3	2.53	0.43
1:D:47:PRO:HB2	1:D:88:ILE:HD11	2.01	0.43
1:A:153:ALA:O	1:A:157:VAL:HG22	2.17	0.43
1:A:57:TYR:HA	1:A:60:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:HIS:O	1:E:81:PHE:HB3	2.18	0.43
1:D:38:TYR:HE2	1:D:69:SER:HB2	1.83	0.43
1:E:151:ILE:O	1:E:154:ALA:N	2.46	0.43
1:E:63:LEU:HB2	1:E:155:GLN:NE2	2.34	0.43
1:E:62:LYS:HB3	1:E:63:LEU:H	1.08	0.43
1:D:14:ALA:HB2	1:D:96:ILE:HG12	2.00	0.43
1:D:16:LYS:N	1:D:79:LYS:HE3	2.35	0.42
1:A:44:PHE:CE1	1:A:47:PRO:HD3	2.55	0.42
1:B:120:ALA:HB2	1:B:135:VAL:HG13	2.02	0.42
1:D:15:PHE:CD1	1:D:79:LYS:HG3	2.52	0.42
1:E:153:ALA:HA	1:E:156:TYR:H	1.83	0.42
1:E:146:ASP:CB	1:E:149:ARG:CB	2.86	0.42
1:C:56:HIS:CD2	1:C:148:LEU:HD12	2.43	0.42
1:D:129:ILE:HD12	1:D:129:ILE:HG23	1.68	0.42
1:E:16:LYS:HZ2	1:E:94:ALA:HB2	1.82	0.42
1:C:139:GLY:HA3	1:D:157:VAL:HG11	2.02	0.42
1:A:91:ILE:HG23	1:A:93:TYR:CZ	2.54	0.42
1:B:61:GLN:HA	1:B:61:GLN:HE21	1.85	0.42
1:E:147:LEU:O	1:E:149:ARG:O	2.38	0.42
1:E:149:ARG:N	1:E:150:LYS:HZ2	2.17	0.42
1:B:20:PHE:CE1	1:B:79:LYS:CE	3.02	0.42
1:D:24:THR:OG1	1:D:26:LYS:HG2	2.20	0.42
1:D:18:GLY:H	1:D:79:LYS:NZ	2.16	0.41
1:A:24:THR:OG1	1:A:26:LYS:CG	2.68	0.41
1:E:156:TYR:O	1:E:157:VAL:C	2.59	0.41
1:E:57:TYR:O	1:E:60:LEU:N	2.54	0.41
1:A:44:PHE:O	1:A:44:PHE:CD2	2.74	0.41
1:C:153:ALA:O	1:C:157:VAL:HG22	2.21	0.41
1:D:15:PHE:C	1:D:79:LYS:HE3	2.41	0.40
1:A:160:HIS:N	1:A:161:PRO:HD3	2.36	0.40
1:E:15:PHE:CE1	1:E:79:LYS:HE3	2.48	0.40
1:E:153:ALA:C	1:E:156:TYR:H	2.24	0.40
1:D:37:PHE:CE2	1:D:104:THR:HA	2.56	0.40
1:D:159:ALA:C	1:D:161:PRO:HD3	2.41	0.40
1:E:62:LYS:HB3	1:E:63:LEU:CD2	2.43	0.40
1:A:58:GLU:HG2	1:A:61:GLN:CB	2.52	0.40
1:D:68:TYR:CD1	1:D:96:ILE:HD11	2.57	0.40
1:D:68:TYR:HB3	1:D:96:ILE:HD12	2.02	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	162/186 (87%)	156 (96%)	6 (4%)	0	100	100
1	B	162/186 (87%)	156 (96%)	4 (2%)	2 (1%)	16	56
1	C	160/186 (86%)	155 (97%)	5 (3%)	0	100	100
1	D	161/186 (87%)	156 (97%)	4 (2%)	1 (1%)	30	70
1	E	160/186 (86%)	147 (92%)	8 (5%)	5 (3%)	5	35
All	All	805/930 (87%)	770 (96%)	27 (3%)	8 (1%)	19	60

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	86	GLU
1	E	62	LYS
1	E	152	LYS
1	E	155	GLN
1	E	48	THR
1	E	153	ALA
1	B	161	PRO
1	D	161	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	137/154 (89%)	134 (98%)	3 (2%)	60	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	136/154 (88%)	134 (98%)	2 (2%)	72	89
1	C	135/154 (88%)	135 (100%)	0	100	100
1	D	136/154 (88%)	134 (98%)	2 (2%)	72	89
1	E	135/154 (88%)	130 (96%)	5 (4%)	41	76
All	All	679/770 (88%)	667 (98%)	12 (2%)	66	87

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	79	LYS
1	A	90	LYS
1	B	4	ASN
1	B	152	LYS
1	D	26	LYS
1	D	71	SER
1	E	4	ASN
1	E	46	CYS
1	E	48	THR
1	E	63	LEU
1	E	79	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	B	17	ASN
1	E	17	ASN
1	E	82	HIS
1	E	155	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 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, 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	163/186 (87%)	0.68	2 (1%) 81 81	38, 62, 105, 169	0
1	B	163/186 (87%)	0.71	2 (1%) 81 81	41, 69, 112, 166	0
1	C	162/186 (87%)	0.94	14 (8%) 13 13	45, 74, 118, 142	0
1	D	162/186 (87%)	1.12	17 (10%) 8 8	62, 84, 125, 169	0
1	E	162/186 (87%)	1.33	45 (27%) 1 1	73, 114, 168, 213	0
All	All	812/930 (87%)	0.95	80 (9%) 9 10	38, 80, 144, 213	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	50	LEU	4.9
1	E	60	LEU	4.2
1	E	63	LEU	4.0
1	E	93	TYR	3.8
1	E	13	GLN	3.7
1	E	132	ALA	3.6
1	E	123	VAL	3.6
1	E	95	MET	3.5
1	E	15	PHE	3.5
1	B	1	SER	3.5
1	D	1	SER	3.5
1	E	50	LEU	3.4
1	E	130	ILE	3.4
1	E	147	LEU	3.4
1	E	28	THR	3.2
1	E	14	ALA	3.0
1	C	1	SER	2.8
1	D	103	LEU	2.8
1	E	16	LYS	2.8
1	C	65	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	32	TRP	2.7
1	E	67	VAL	2.7
1	E	88	ILE	2.7
1	E	94	ALA	2.7
1	E	35	PHE	2.7
1	C	130	ILE	2.7
1	E	53	VAL	2.7
1	C	123	VAL	2.7
1	C	131	GLN	2.7
1	E	124	VAL	2.6
1	C	32	TRP	2.6
1	E	17	ASN	2.6
1	E	23	VAL	2.6
1	E	46	CYS	2.6
1	D	122	PHE	2.5
1	E	92	LYS	2.5
1	E	68	TYR	2.5
1	E	36	PHE	2.5
1	D	140	ILE	2.5
1	D	7	ILE	2.5
1	C	35	PHE	2.5
1	E	54	ALA	2.4
1	D	123	VAL	2.4
1	E	90	LYS	2.4
1	E	107	PHE	2.4
1	D	104	THR	2.3
1	D	135	VAL	2.3
1	E	110	MET	2.3
1	E	131	GLN	2.3
1	D	93	TYR	2.3
1	E	57	TYR	2.3
1	E	96	ILE	2.3
1	E	10	PHE	2.3
1	E	43	THR	2.2
1	E	3	ILE	2.2
1	E	122	PHE	2.2
1	E	22	GLU	2.2
1	D	91	ILE	2.2
1	D	47	PRO	2.2
1	C	140	ILE	2.2
1	C	155	GLN	2.2
1	E	155	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	148	LEU	2.2
1	C	63	LEU	2.1
1	D	4[A]	ASN	2.1
1	D	95	MET	2.1
1	E	2	LEU	2.1
1	E	4	ASN	2.1
1	E	21	ILE	2.1
1	C	60	LEU	2.1
1	E	51	GLY	2.1
1	C	5	THR	2.1
1	D	111	ARG	2.1
1	A	91	ILE	2.0
1	C	151	ILE	2.0
1	D	81	PHE	2.0
1	E	103	LEU	2.0
1	B	79	LYS	2.0
1	A	140	ILE	2.0
1	D	142	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 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	K	D	201	1/1	0.96	0.40	1.12	118,118,118,118	0
2	K	A	201	1/1	0.96	0.28	-0.55	48,48,48,48	1
2	K	B	201	1/1	0.89	0.15	-2.41	83,83,83,83	0
2	K	B	202	1/1	0.95	0.20	-	71,71,71,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.