Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 07:27 pm BST

PDB ID	:	3B4S
Title	:	Crystal structure of a LuxT domain from Vibrio parahaemolyticus RIMD 2210633
Authors	:	Tan, K.; Zhou, M.; Gu, M.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2007-10-24
Resolution	:	3.10 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

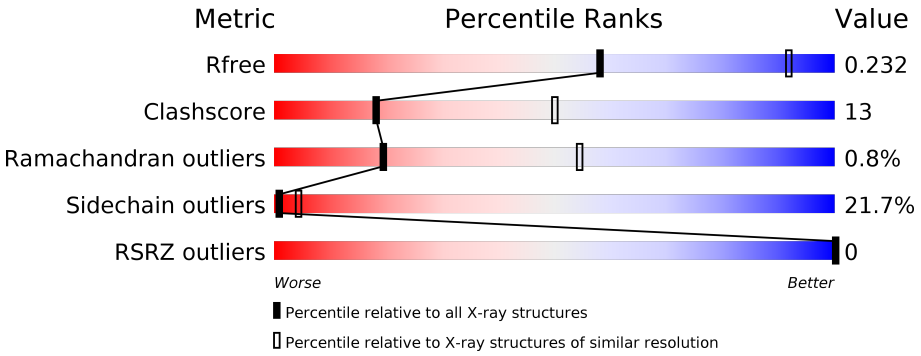
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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 <=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	94	66% 28% • •
1	B	94	68% 22% 6% •
1	C	94	52% 39% 6% •
1	D	94	59% 31% 6% •
1	E	94	66% 20% 11% •
1	F	94	69% 19% 6% • •

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Mol	Chain	Length	Quality of chain
1	G	94	
1	H	94	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5906 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 Protein LuxT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	92	Total	C	N	O	Se	0	0	0
			745	481	124	137	3			
1	B	91	Total	C	N	O	Se	0	0	0
			740	478	123	136	3			
1	C	92	Total	C	N	O	Se	0	0	0
			745	481	124	137	3			
1	D	90	Total	C	N	O	Se	0	0	0
			732	474	122	133	3			
1	E	91	Total	C	N	O	Se	0	0	0
			740	478	123	136	3			
1	F	90	Total	C	N	O	Se	0	0	0
			732	474	122	133	3			
1	G	91	Total	C	N	O	Se	0	0	0
			740	478	123	136	3			
1	H	90	Total	C	N	O	Se	0	0	0
			732	474	122	133	3			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	SER	-	EXPRESSION TAG	UNP Q87J33
A	61	ASN	-	EXPRESSION TAG	UNP Q87J33
A	62	ALA	-	EXPRESSION TAG	UNP Q87J33
B	60	SER	-	EXPRESSION TAG	UNP Q87J33
B	61	ASN	-	EXPRESSION TAG	UNP Q87J33
B	62	ALA	-	EXPRESSION TAG	UNP Q87J33
C	60	SER	-	EXPRESSION TAG	UNP Q87J33
C	61	ASN	-	EXPRESSION TAG	UNP Q87J33
C	62	ALA	-	EXPRESSION TAG	UNP Q87J33
D	60	SER	-	EXPRESSION TAG	UNP Q87J33
D	61	ASN	-	EXPRESSION TAG	UNP Q87J33
D	62	ALA	-	EXPRESSION TAG	UNP Q87J33
E	60	SER	-	EXPRESSION TAG	UNP Q87J33

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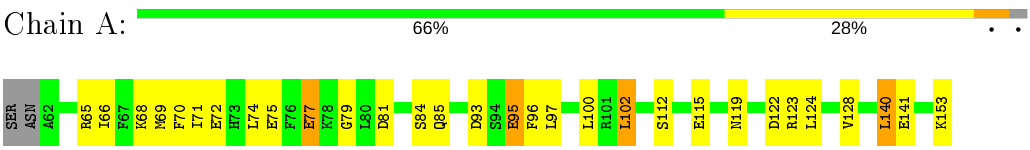
Chain	Residue	Modelled	Actual	Comment	Reference
E	61	ASN	-	EXPRESSION TAG	UNP Q87J33
E	62	ALA	-	EXPRESSION TAG	UNP Q87J33
F	60	SER	-	EXPRESSION TAG	UNP Q87J33
F	61	ASN	-	EXPRESSION TAG	UNP Q87J33
F	62	ALA	-	EXPRESSION TAG	UNP Q87J33
G	60	SER	-	EXPRESSION TAG	UNP Q87J33
G	61	ASN	-	EXPRESSION TAG	UNP Q87J33
G	62	ALA	-	EXPRESSION TAG	UNP Q87J33
H	60	SER	-	EXPRESSION TAG	UNP Q87J33
H	61	ASN	-	EXPRESSION TAG	UNP Q87J33
H	62	ALA	-	EXPRESSION TAG	UNP Q87J33

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

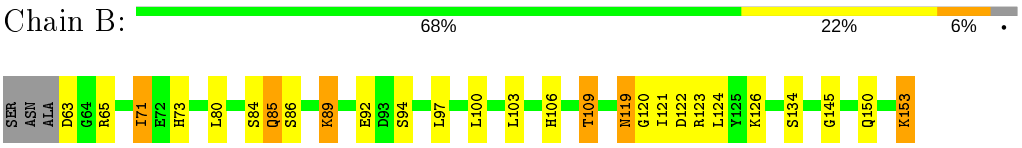
- Molecule 1: Protein LuxT

Chain A:



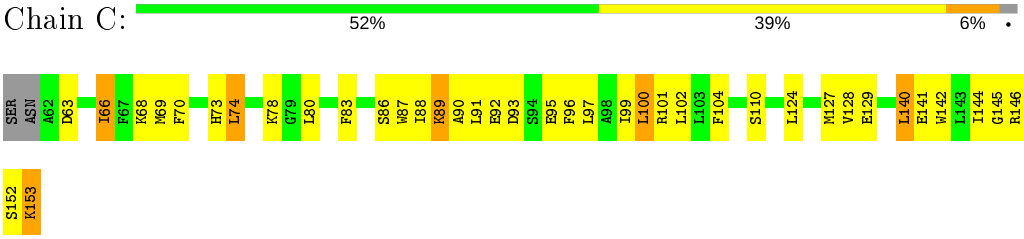
- Molecule 1: Protein LuxT

Chain B:



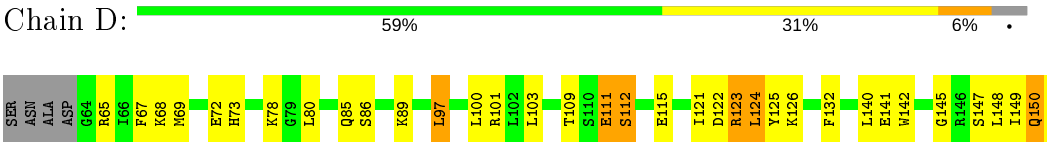
- Molecule 1: Protein LuxT

Chain C:



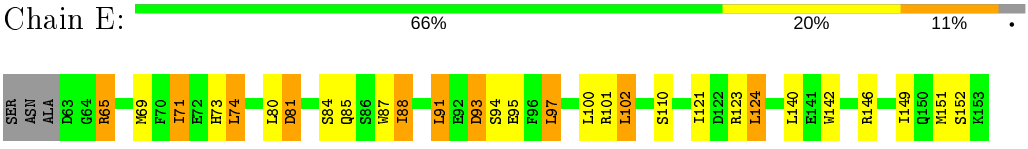
- Molecule 1: Protein LuxT

Chain D:



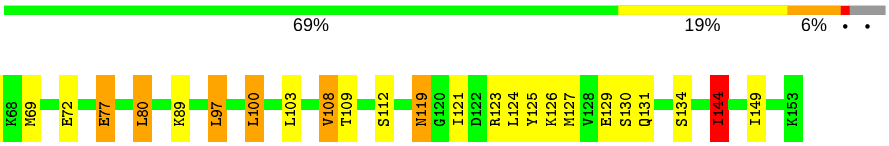
- Molecule 1: Protein LuxT

Chain E:



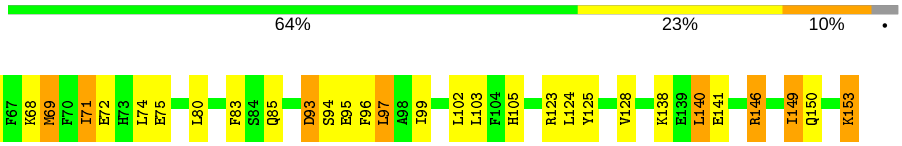
- Molecule 1: Protein LuxT

Chain F:



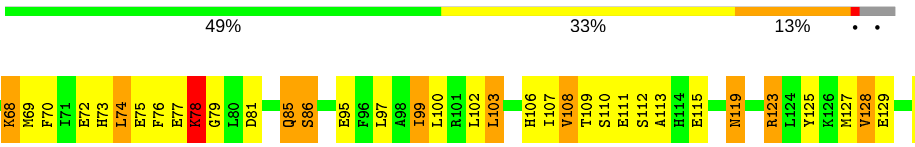
• Molecule 1: Protein LuxT

Chain G:



• Molecule 1: Protein LuxT

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	147.44Å 147.44Å 382.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.22 – 3.10 48.22 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.22-3.10) 99.8 (48.22-3.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.33 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.190 , 0.232 0.188 , 0.232	Depositor DCC
R_{free} test set	1490 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	71.4	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 27.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5906	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.88	1/758 (0.1%)	0.94	1/1009 (0.1%)
1	B	0.89	0/753	0.92	0/1002
1	C	0.86	0/758	0.86	0/1009
1	D	0.88	0/745	0.84	0/991
1	E	0.86	0/753	0.88	1/1002 (0.1%)
1	F	0.86	1/745 (0.1%)	0.88	0/991
1	G	0.83	0/753	0.91	1/1002 (0.1%)
1	H	0.83	0/745	0.86	0/991
All	All	0.86	2/6010 (0.0%)	0.89	3/7997 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	ARG	CG-CD	5.58	1.65	1.51
1	F	144	ILE	CA-CB	5.22	1.66	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	123	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	A	102	LEU	CB-CG-CD1	-5.91	100.95	111.00
1	E	91	LEU	CA-CB-CG	5.74	128.51	115.30

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	745	0	730	18	0
1	B	740	0	725	13	0
1	C	745	0	730	29	0
1	D	732	0	721	28	0
1	E	740	0	725	21	0
1	F	732	0	721	21	0
1	G	740	0	725	22	0
1	H	732	0	721	45	0
All	All	5906	0	5798	157	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 13.

All (157) 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:G:153:LYS:HA	1:G:153:LYS:HE3	1.29	1.10
1:A:119:ASN:ND2	1:A:122:ASP:H	1.68	0.91
1:C:83:PHE:O	1:C:86:SER:HB3	1.71	0.90
1:F:69:MSE:HA	1:F:72:GLU:HG2	1.54	0.89
1:B:119:ASN:HD22	1:B:119:ASN:C	1.78	0.85
1:C:127:MSE:SE	1:G:71:ILE:HD11	2.27	0.84
1:G:153:LYS:CE	1:G:153:LYS:HA	2.10	0.80
1:B:89:LYS:HE3	1:B:92:GLU:OE1	1.84	0.78
1:F:77:GLU:HA	1:F:77:GLU:OE2	1.85	0.77
1:A:119:ASN:HD21	1:A:122:ASP:H	1.33	0.76
1:F:69:MSE:HA	1:F:72:GLU:CG	2.17	0.75
1:A:69:MSE:HE3	1:A:95:GLU:OE1	1.87	0.75
1:D:67:PHE:CZ	1:H:127:MSE:HE1	2.28	0.69
1:C:128:VAL:HG21	1:C:140:LEU:HG	1.74	0.69
1:A:85:GLN:OE1	1:A:85:GLN:HA	1.93	0.67
1:E:152:SER:HB3	1:H:107:ILE:HD13	1.77	0.66
1:F:119:ASN:HD22	1:F:123:ARG:HG3	1.61	0.66
1:G:95:GLU:O	1:G:99:ILE:HG13	1.96	0.66
1:F:77:GLU:OE2	1:F:77:GLU:CA	2.44	0.65
1:A:66:ILE:HG12	1:B:73:HIS:CE1	2.33	0.64
1:C:69:MSE:HE3	1:C:95:GLU:OE1	1.99	0.63
1:E:94:SER:HA	1:E:97:LEU:HB2	1.79	0.63
1:F:119:ASN:ND2	1:F:123:ARG:HG3	2.14	0.63
1:F:144:ILE:C	1:F:144:ILE:HD12	2.19	0.63
1:E:65:ARG:HG3	1:E:69:MSE:CE	2.29	0.62
1:C:69:MSE:HE1	1:D:69:MSE:HG3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:VAL:HG21	1:A:140:LEU:HG	1.82	0.61
1:B:119:ASN:ND2	1:B:119:ASN:C	2.52	0.61
1:D:67:PHE:HZ	1:H:127:MSE:CE	2.13	0.60
1:H:68:LYS:O	1:H:72:GLU:HG3	2.00	0.60
1:B:106:HIS:O	1:B:109:THR:HB	2.01	0.60
1:C:100:LEU:HB3	1:E:151:MSE:HE1	1.84	0.59
1:H:128:VAL:HG13	1:H:136:GLY:C	2.24	0.58
1:H:77:GLU:O	1:H:79:GLY:N	2.35	0.58
1:C:141:GLU:O	1:D:145:GLY:HA3	2.02	0.58
1:D:67:PHE:CE1	1:H:127:MSE:HE1	2.39	0.58
1:G:68:LYS:O	1:G:72:GLU:HG2	2.03	0.58
1:D:68:LYS:O	1:D:72:GLU:HG3	2.03	0.58
1:C:101:ARG:HG2	1:H:110:SER:OG	2.04	0.58
1:D:132:PHE:CD1	1:F:80:LEU:HD13	2.41	0.56
1:H:106:HIS:O	1:H:109:THR:HG22	2.06	0.55
1:C:74:LEU:HA	1:C:86:SER:OG	2.06	0.55
1:G:99:ILE:O	1:G:103:LEU:HG	2.07	0.55
1:G:93:ASP:OD1	1:G:93:ASP:C	2.45	0.54
1:H:70:PHE:HB2	1:H:99:ILE:HD11	1.89	0.54
1:C:63:ASP:OD1	1:E:123:ARG:HD3	2.06	0.54
1:D:111:GLU:CD	1:D:111:GLU:H	2.12	0.54
1:G:149:ILE:HG22	1:G:150:GLN:N	2.23	0.54
1:H:125:TYR:O	1:H:129:GLU:HG2	2.08	0.54
1:C:150:GLN:O	1:C:150:GLN:HG2	2.06	0.53
1:A:66:ILE:HG12	1:B:73:HIS:HE1	1.70	0.53
1:B:121:ILE:C	1:B:121:ILE:HD12	2.29	0.53
1:E:87:TRP:CD1	1:E:91:LEU:HD22	2.44	0.53
1:E:65:ARG:HG3	1:E:69:MSE:HE2	1.89	0.52
1:H:111:GLU:O	1:H:111:GLU:OE1	2.27	0.52
1:C:97:LEU:HD23	1:E:151:MSE:HE2	1.92	0.51
1:F:126:LYS:O	1:F:129:GLU:HB3	2.11	0.51
1:D:67:PHE:CZ	1:H:127:MSE:CE	2.91	0.51
1:C:89:LYS:O	1:C:92:GLU:HG2	2.11	0.51
1:C:73:HIS:HE1	1:C:95:GLU:OE2	1.94	0.50
1:E:81:ASP:OD1	1:E:81:ASP:N	2.44	0.50
1:F:121:ILE:HG23	1:H:103:LEU:HD22	1.92	0.50
1:F:108:VAL:CG1	1:G:105:HIS:HA	2.41	0.50
1:F:112:SER:HB3	1:H:65:ARG:H	1.77	0.50
1:H:140:LEU:O	1:H:144:ILE:HG12	2.12	0.50
1:B:85:GLN:HA	1:B:85:GLN:OE1	2.11	0.50
1:H:119:ASN:HB2	1:H:123:ARG:HE	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:128:VAL:HG21	1:G:140:LEU:HG	1.94	0.49
1:E:95:GLU:HG3	1:F:69:MSE:HE1	1.95	0.49
1:H:74:LEU:HA	1:H:86:SER:OG	2.13	0.48
1:E:152:SER:CB	1:H:107:ILE:HD13	2.43	0.48
1:G:125:TYR:HD1	1:H:149:ILE:HD12	1.77	0.48
1:A:115:GLU:OE2	1:A:115:GLU:HA	2.14	0.48
1:H:65:ARG:O	1:H:68:LYS:HB3	2.14	0.48
1:A:93:ASP:OD1	1:A:93:ASP:C	2.52	0.47
1:D:150:GLN:HA	1:D:150:GLN:OE1	2.14	0.47
1:H:144:ILE:O	1:H:147:SER:HB2	2.13	0.47
1:B:153:LYS:HE2	1:B:153:LYS:HB3	1.55	0.47
1:C:104:PHE:HB3	1:H:108:VAL:CG2	2.44	0.47
1:D:124:LEU:HD13	1:D:140:LEU:HD11	1.96	0.47
1:F:125:TYR:O	1:F:129:GLU:HB2	2.15	0.47
1:C:144:ILE:O	1:C:147:SER:HB2	2.14	0.47
1:C:152:SER:O	1:C:153:LYS:CB	2.62	0.47
1:E:87:TRP:HD1	1:E:91:LEU:HD22	1.79	0.47
1:H:70:PHE:HB2	1:H:99:ILE:CD1	2.45	0.47
1:H:69:MSE:O	1:H:72:GLU:HB2	2.15	0.46
1:D:85:GLN:CA	1:D:85:GLN:NE2	2.77	0.46
1:E:73:HIS:NE2	1:E:93:ASP:OD2	2.48	0.46
1:D:85:GLN:NE2	1:D:85:GLN:HA	2.30	0.46
1:A:66:ILE:HA	1:A:66:ILE:HD13	1.70	0.46
1:G:141:GLU:O	1:H:145:GLY:HA3	2.15	0.46
1:F:108:VAL:HG13	1:G:105:HIS:HA	1.98	0.46
1:D:147:SER:O	1:D:150:GLN:HB2	2.15	0.46
1:H:81:ASP:O	1:H:85:GLN:HB2	2.15	0.46
1:B:119:ASN:HD22	1:B:120:GLY:N	2.13	0.46
1:A:119:ASN:HD21	1:A:122:ASP:N	2.08	0.46
1:A:77:GLU:O	1:A:79:GLY:N	2.49	0.46
1:A:69:MSE:CE	1:A:95:GLU:OE1	2.61	0.46
1:C:70:PHE:CE2	1:C:96:PHE:CE1	3.04	0.45
1:C:87:TRP:O	1:C:90:ALA:N	2.49	0.45
1:E:73:HIS:HE1	1:E:95:GLU:OE2	1.99	0.45
1:A:93:ASP:OD1	1:A:95:GLU:N	2.50	0.44
1:D:124:LEU:HD23	1:D:124:LEU:HA	1.81	0.44
1:H:111:GLU:O	1:H:113:ALA:N	2.50	0.44
1:D:85:GLN:HE21	1:D:85:GLN:N	2.15	0.44
1:D:67:PHE:HZ	1:H:127:MSE:HE3	1.81	0.44
1:D:69:MSE:HE3	1:D:69:MSE:HB2	1.83	0.44
1:A:68:LYS:HE3	1:A:68:LYS:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:93:ASP:OD1	1:G:94:SER:N	2.51	0.44
1:D:97:LEU:HA	1:D:97:LEU:HD12	1.68	0.44
1:G:66:ILE:HB	1:H:73:HIS:CE1	2.53	0.44
1:H:111:GLU:C	1:H:113:ALA:H	2.21	0.43
1:G:125:TYR:CD1	1:H:149:ILE:HD12	2.53	0.43
1:H:128:VAL:HG13	1:H:136:GLY:O	2.19	0.43
1:E:121:ILE:HA	1:E:121:ILE:HD13	1.87	0.42
1:A:70:PHE:CE2	1:A:96:PHE:CE1	3.08	0.42
1:G:66:ILE:O	1:G:69:MSE:HB2	2.19	0.42
1:C:142:TRP:HA	1:D:142:TRP:HA	2.02	0.42
1:H:128:VAL:HG13	1:H:136:GLY:CA	2.50	0.42
1:H:95:GLU:O	1:H:99:ILE:HG23	2.19	0.42
1:C:127:MSE:HE2	1:C:127:MSE:HB3	1.77	0.42
1:C:95:GLU:HA	1:D:65:ARG:HD3	2.01	0.42
1:G:146:ARG:HD3	1:G:146:ARG:HA	1.74	0.42
1:H:150:GLN:HA	1:H:150:GLN:HE21	1.85	0.42
1:A:66:ILE:CG1	1:B:73:HIS:HE1	2.31	0.42
1:C:145:GLY:HA3	1:D:141:GLU:O	2.19	0.42
1:E:88:ILE:HA	1:E:91:LEU:CD2	2.50	0.42
1:F:100:LEU:HD12	1:F:100:LEU:HA	1.82	0.42
1:H:100:LEU:HD12	1:H:100:LEU:HA	1.90	0.42
1:C:66:ILE:HD11	1:D:73:HIS:HE1	1.85	0.41
1:F:80:LEU:HD12	1:F:80:LEU:HA	1.68	0.41
1:H:78:LYS:O	1:H:78:LYS:HG3	2.21	0.41
1:C:95:GLU:O	1:C:99:ILE:HG13	2.20	0.41
1:D:148:LEU:O	1:D:149:ILE:C	2.58	0.41
1:H:111:GLU:OE1	1:H:111:GLU:HA	2.20	0.41
1:A:141:GLU:O	1:B:145:GLY:HA3	2.20	0.41
1:F:127:MSE:HE2	1:H:76:PHE:CE2	2.55	0.41
1:E:102:LEU:HD22	1:E:102:LEU:HA	1.76	0.41
1:C:127:MSE:SE	1:G:71:ILE:CD1	3.09	0.41
1:C:91:LEU:HD12	1:C:91:LEU:HA	1.83	0.41
1:G:96:PHE:O	1:G:97:LEU:C	2.57	0.41
1:E:65:ARG:HD2	1:E:69:MSE:HE2	2.02	0.41
1:E:142:TRP:CZ2	1:E:146:ARG:HD3	2.56	0.41
1:D:151:MSE:HE2	1:F:97:LEU:HD12	2.02	0.41
1:H:111:GLU:C	1:H:113:ALA:N	2.75	0.41
1:F:121:ILE:HG22	1:H:103:LEU:HD13	2.03	0.40
1:H:119:ASN:HD22	1:H:123:ARG:HH21	1.70	0.40
1:G:65:ARG:HB3	1:H:73:HIS:CD2	2.57	0.40
1:E:124:LEU:HA	1:E:124:LEU:HD23	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:ILE:O	1:E:74:LEU:HB2	2.22	0.40
1:H:69:MSE:HA	1:H:72:GLU:HG3	2.04	0.40
1:B:71:ILE:HD13	1:B:71:ILE:HA	1.80	0.40
1:C:66:ILE:HD11	1:D:73:HIS:CE1	2.56	0.40
1:D:100:LEU:HD23	1:D:100:LEU:HA	1.90	0.40
1:D:123:ARG:HB2	1:F:67:PHE:CZ	2.56	0.40
1:G:80:LEU:O	1:G:83:PHE:HB3	2.21	0.40
1:C:100:LEU:HD23	1:C:100:LEU:HA	1.75	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	90/94 (96%)	84 (93%)	5 (6%)	1 (1%)	14 46
1	B	89/94 (95%)	84 (94%)	5 (6%)	0	100 100
1	C	90/94 (96%)	83 (92%)	6 (7%)	1 (1%)	14 46
1	D	88/94 (94%)	79 (90%)	7 (8%)	2 (2%)	6 28
1	E	89/94 (95%)	85 (96%)	4 (4%)	0	100 100
1	F	88/94 (94%)	78 (89%)	10 (11%)	0	100 100
1	G	89/94 (95%)	84 (94%)	5 (6%)	0	100 100
1	H	88/94 (94%)	81 (92%)	5 (6%)	2 (2%)	6 28
All	All	711/752 (94%)	658 (92%)	47 (7%)	6 (1%)	19 54

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	78	LYS
1	D	112	SER

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Mol	Chain	Res	Type
1	H	112	SER
1	A	77	GLU
1	D	115	GLU
1	C	88	ILE

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	78/77 (101%)	63 (81%)	15 (19%)	1	6
1	B	78/77 (101%)	57 (73%)	21 (27%)	0	1
1	C	78/77 (101%)	61 (78%)	17 (22%)	1	4
1	D	77/77 (100%)	60 (78%)	17 (22%)	1	4
1	E	78/77 (101%)	61 (78%)	17 (22%)	1	4
1	F	77/77 (100%)	62 (80%)	15 (20%)	1	6
1	G	78/77 (101%)	63 (81%)	15 (19%)	1	6
1	H	77/77 (100%)	59 (77%)	18 (23%)	1	3
All	All	621/616 (101%)	486 (78%)	135 (22%)	1	4

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ARG
1	A	71	ILE
1	A	72	GLU
1	A	74	LEU
1	A	75	GLU
1	A	81	ASP
1	A	84	SER
1	A	95	GLU
1	A	97	LEU
1	A	100	LEU
1	A	102	LEU

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Mol	Chain	Res	Type
1	A	112	SER
1	A	124	LEU
1	A	140	LEU
1	A	153	LYS
1	B	63	ASP
1	B	65	ARG
1	B	71	ILE
1	B	80	LEU
1	B	84	SER
1	B	85	GLN
1	B	86	SER
1	B	89	LYS
1	B	94	SER
1	B	97	LEU
1	B	100	LEU
1	B	103	LEU
1	B	109	THR
1	B	119	ASN
1	B	122	ASP
1	B	123	ARG
1	B	124	LEU
1	B	126	LYS
1	B	134	SER
1	B	150	GLN
1	B	153	LYS
1	C	66	ILE
1	C	68	LYS
1	C	74	LEU
1	C	78	LYS
1	C	80	LEU
1	C	89	LYS
1	C	93	ASP
1	C	100	LEU
1	C	102	LEU
1	C	110	SER
1	C	124	LEU
1	C	129	GLU
1	C	140	LEU
1	C	146	ARG
1	C	148	LEU
1	C	149	ILE
1	C	153	LYS

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Mol	Chain	Res	Type
1	D	78	LYS
1	D	80	LEU
1	D	86	SER
1	D	89	LYS
1	D	97	LEU
1	D	101	ARG
1	D	103	LEU
1	D	109	THR
1	D	111	GLU
1	D	112	SER
1	D	121	ILE
1	D	122	ASP
1	D	123	ARG
1	D	124	LEU
1	D	125	TYR
1	D	126	LYS
1	D	150	GLN
1	E	65	ARG
1	E	71	ILE
1	E	74	LEU
1	E	80	LEU
1	E	81	ASP
1	E	84	SER
1	E	85	GLN
1	E	88	ILE
1	E	93	ASP
1	E	97	LEU
1	E	100	LEU
1	E	101	ARG
1	E	102	LEU
1	E	110	SER
1	E	124	LEU
1	E	140	LEU
1	E	149	ILE
1	F	77	GLU
1	F	80	LEU
1	F	89	LYS
1	F	97	LEU
1	F	100	LEU
1	F	103	LEU
1	F	108	VAL
1	F	109	THR

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Mol	Chain	Res	Type
1	F	119	ASN
1	F	124	LEU
1	F	130	SER
1	F	131	GLN
1	F	134	SER
1	F	144	ILE
1	F	149	ILE
1	G	65	ARG
1	G	69	MSE
1	G	71	ILE
1	G	74	LEU
1	G	75	GLU
1	G	85	GLN
1	G	93	ASP
1	G	97	LEU
1	G	102	LEU
1	G	124	LEU
1	G	138	LYS
1	G	140	LEU
1	G	146	ARG
1	G	149	ILE
1	G	153	LYS
1	H	65	ARG
1	H	68	LYS
1	H	74	LEU
1	H	75	GLU
1	H	78	LYS
1	H	85	GLN
1	H	86	SER
1	H	97	LEU
1	H	99	ILE
1	H	102	LEU
1	H	103	LEU
1	H	108	VAL
1	H	115	GLU
1	H	119	ASN
1	H	123	ARG
1	H	128	VAL
1	H	138	LYS
1	H	140	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	HIS
1	A	119	ASN
1	B	73	HIS
1	B	119	ASN
1	C	73	HIS
1	D	73	HIS
1	D	85	GLN
1	F	85	GLN
1	F	119	ASN
1	F	131	GLN
1	G	85	GLN
1	H	73	HIS
1	H	119	ASN
1	H	150	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

There are no ligands in this entry.

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^{th} 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	89/94 (94%)	-0.30	0	100	100	46, 59, 81, 96	0
1	B	88/94 (93%)	-0.33	0	100	100	45, 62, 80, 104	0
1	C	89/94 (94%)	-0.37	0	100	100	56, 64, 80, 100	0
1	D	87/94 (92%)	-0.14	0	100	100	53, 70, 108, 113	0
1	E	88/94 (93%)	-0.27	0	100	100	49, 65, 86, 91	0
1	F	87/94 (92%)	-0.33	0	100	100	51, 73, 97, 100	0
1	G	88/94 (93%)	-0.51	0	100	100	50, 70, 91, 102	0
1	H	87/94 (92%)	-0.20	0	100	100	49, 70, 99, 109	0
All	All	703/752 (93%)	-0.31	0	100	100	45, 67, 95, 113	0

There are no RSRZ outliers to report.

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 carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.