



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:40 pm GMT

PDB ID : 1QOH  
Title : A MUTANT SHIGA-LIKE TOXIN IIE  
Authors : Pannu, N.S.; Boodhoo, A.; Armstrong, G.D.; Clark, C.G.; Brunton, J.L.;  
Read, R.J.  
Deposited on : 1999-11-08  
Resolution : 2.35 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
Xtrriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

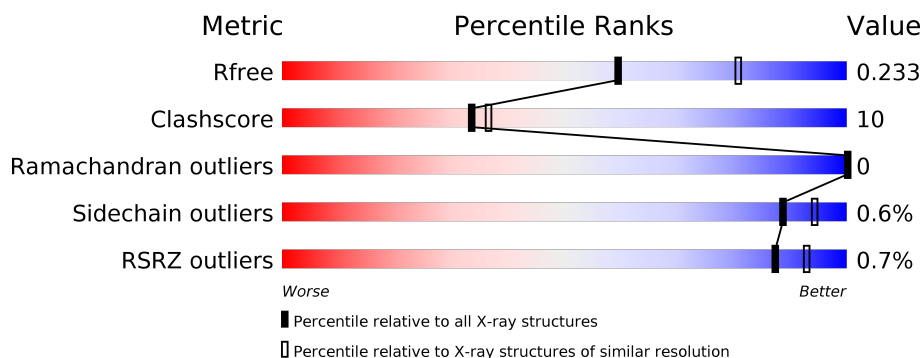
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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.






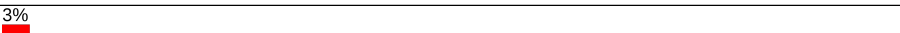

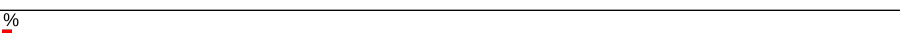


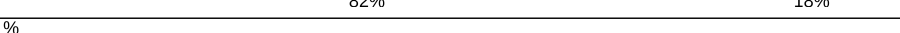




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1522 (2.38-2.34)
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)
RSRZ outliers	101464	1528 (2.38-2.34)

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	68	<div> <div>85%</div> <div>13%</div> <div>.</div> </div>
1	B	68	<div> <div>%</div> <div>88%</div> <div>12%</div> </div>
1	C	68	<div> <div>3%</div> <div>79%</div> <div>19%</div> <div>.</div> </div>
1	D	68	<div> <div>87%</div> <div>13%</div> </div>
1	E	68	<div> <div>90%</div> <div>10%</div> </div>
1	F	68	<div> <div>%</div> <div>87%</div> <div>13%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	68	 78%21%.
1	H	68	 %88%12%
1	I	68	 87%13%
1	J	68	 82%18%
1	K	68	 3%90%10%
1	L	68	 87%13%
1	M	68	 %84%16%
1	N	68	 87%12%.
1	O	68	 82%18%
1	P	68	 %84%16%
1	Q	68	 84%16%
1	R	68	 91%9%
1	S	68	 90%10%
1	T	68	 91%9%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11019 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 SHIGA-LIKE TOXIN IIE B SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	68	Total	C	N	O	S	0	0	0
			533	333	90	107	3			
1	B	68	Total	C	N	O	S	0	0	0
			533	333	90	107	3			
1	C	68	Total	C	N	O	S	0	0	0
			533	333	90	107	3			
1	D	68	Total	C	N	O	S	0	0	0
			533	333	90	107	3			
1	E	68	Total	C	N	O	S	0	0	0
			533	333	90	107	3			
1	F	68	Total	C	N	O	S	0	0	0
			533	333	90	107	3			
1	G	68	Total	C	N	O	S	0	0	0
			533	333	90	107	3			
1	H	68	Total	C	N	O	S	0	0	0
			533	333	90	107	3			
1	I	68	Total	C	N	O	S	0	0	0
			533	333	90	107	3			
1	J	68	Total	C	N	O	S	0	0	0
			533	333	90	107	3			
1	K	68	Total	C	N	O	S	0	0	0
			533	333	90	107	3			
1	L	68	Total	C	N	O	S	0	0	0
			533	333	90	107	3			
1	M	68	Total	C	N	O	S	0	0	0
			533	333	90	107	3			
1	N	68	Total	C	N	O	S	0	0	0
			533	333	90	107	3			
1	O	68	Total	C	N	O	S	0	0	0
			533	333	90	107	3			
1	P	68	Total	C	N	O	S	0	0	0
			533	333	90	107	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	68	Total	C	N	O	S	0	0	0
			533	333	90	107	3			
1	R	68	Total	C	N	O	S	0	0	0
			533	333	90	107	3			
1	S	68	Total	C	N	O	S	0	0	0
			533	333	90	107	3			
1	T	68	Total	C	N	O	S	0	0	0
			533	333	90	107	3			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	165	GLU	GLN	ENGINEERED MUTATION	UNP Q47644
A	167	GLN	LYS	ENGINEERED MUTATION	UNP Q47644
B	265	GLU	GLN	ENGINEERED MUTATION	UNP Q47644
B	267	GLN	LYS	ENGINEERED MUTATION	UNP Q47644
C	365	GLU	GLN	ENGINEERED MUTATION	UNP Q47644
C	367	GLN	LYS	ENGINEERED MUTATION	UNP Q47644
D	465	GLU	GLN	ENGINEERED MUTATION	UNP Q47644
D	467	GLN	LYS	ENGINEERED MUTATION	UNP Q47644
E	565	GLU	GLN	ENGINEERED MUTATION	UNP Q47644
E	567	GLN	LYS	ENGINEERED MUTATION	UNP Q47644
F	165	GLU	GLN	ENGINEERED MUTATION	UNP Q47644
F	167	GLN	LYS	ENGINEERED MUTATION	UNP Q47644
G	265	GLU	GLN	ENGINEERED MUTATION	UNP Q47644
G	267	GLN	LYS	ENGINEERED MUTATION	UNP Q47644
H	365	GLU	GLN	ENGINEERED MUTATION	UNP Q47644
H	367	GLN	LYS	ENGINEERED MUTATION	UNP Q47644
I	465	GLU	GLN	ENGINEERED MUTATION	UNP Q47644
I	467	GLN	LYS	ENGINEERED MUTATION	UNP Q47644
J	565	GLU	GLN	ENGINEERED MUTATION	UNP Q47644
J	567	GLN	LYS	ENGINEERED MUTATION	UNP Q47644
K	165	GLU	GLN	ENGINEERED MUTATION	UNP Q47644
K	167	GLN	LYS	ENGINEERED MUTATION	UNP Q47644
L	265	GLU	GLN	ENGINEERED MUTATION	UNP Q47644
L	267	GLN	LYS	ENGINEERED MUTATION	UNP Q47644
M	365	GLU	GLN	ENGINEERED MUTATION	UNP Q47644
M	367	GLN	LYS	ENGINEERED MUTATION	UNP Q47644
N	465	GLU	GLN	ENGINEERED MUTATION	UNP Q47644
N	467	GLN	LYS	ENGINEERED MUTATION	UNP Q47644
O	565	GLU	GLN	ENGINEERED MUTATION	UNP Q47644
O	567	GLN	LYS	ENGINEERED MUTATION	UNP Q47644
P	165	GLU	GLN	ENGINEERED MUTATION	UNP Q47644

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Chain	Residue	Modelled	Actual	Comment	Reference
P	167	GLN	LYS	ENGINEERED MUTATION	UNP Q47644
Q	265	GLU	GLN	ENGINEERED MUTATION	UNP Q47644
Q	267	GLN	LYS	ENGINEERED MUTATION	UNP Q47644
R	365	GLU	GLN	ENGINEERED MUTATION	UNP Q47644
R	367	GLN	LYS	ENGINEERED MUTATION	UNP Q47644
S	465	GLU	GLN	ENGINEERED MUTATION	UNP Q47644
S	467	GLN	LYS	ENGINEERED MUTATION	UNP Q47644
T	565	GLU	GLN	ENGINEERED MUTATION	UNP Q47644
T	567	GLN	LYS	ENGINEERED MUTATION	UNP Q47644

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	25	Total O 25 25	0	0
2	B	16	Total O 16 16	0	0
2	C	12	Total O 12 12	0	0
2	D	16	Total O 16 16	0	0
2	E	15	Total O 15 15	0	0
2	F	14	Total O 14 14	0	0
2	G	19	Total O 19 19	0	0
2	H	13	Total O 13 13	0	0
2	I	25	Total O 25 25	0	0
2	J	24	Total O 24 24	0	0
2	K	18	Total O 18 18	0	0
2	L	10	Total O 10 10	0	0
2	M	13	Total O 13 13	0	0
2	N	14	Total O 14 14	0	0
2	O	22	Total O 22 22	0	0

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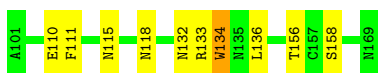
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	20	Total 20	O 20	0	0
2	Q	17	Total 17	O 17	0	0
2	R	19	Total 19	O 19	0	0
2	S	27	Total 27	O 27	0	0
2	T	20	Total 20	O 20	0	0

### 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: SHIGA-LIKE TOXIN IIE B SUBUNIT

Chain A: 




- Molecule 1: SHIGA-LIKE TOXIN IIE B SUBUNIT

Chain B: 



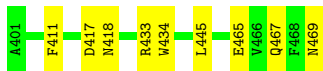
- Molecule 1: SHIGA-LIKE TOXIN IIE B SUBUNIT

Chain C: 



- Molecule 1: SHIGA-LIKE TOXIN IIE B SUBUNIT

Chain D: 




- Molecule 1: SHIGA-LIKE TOXIN IIE B SUBUNIT

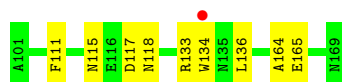
Chain E: 



- Molecule 1: SHIGA-LIKE TOXIN IIE B SUBUNIT

Chain F: 





- Molecule 1: SHIGA-LIKE TOXIN IIE B SUBUNIT

Chain G: 78% 21%



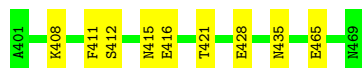
- Molecule 1: SHIGA-LIKE TOXIN IIE B SUBUNIT

Chain H: 88% 12%



- Molecule 1: SHIGA-LIKE TOXIN IIE B SUBUNIT

Chain I: 87% 13%



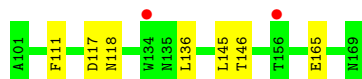
- Molecule 1: SHIGA-LIKE TOXIN IIE B SUBUNIT

Chain J: 82% 18%



- Molecule 1: SHIGA-LIKE TOXIN IIE B SUBUNIT

Chain K: 3% 90% 10%



- Molecule 1: SHIGA-LIKE TOXIN IIE B SUBUNIT

Chain L: 87% 13%




- Molecule 1: SHIGA-LIKE TOXIN IIE B SUBUNIT

Chain M: 84% 16%




## ● Molecule 1: SHIGA-LIKE TOXIN IIE B SUBUNIT

Chain N:  87% 12%


## ● Molecule 1: SHIGA-LIKE TOXIN IIE B SUBUNIT

Chain O:  82% 18%

## ● Molecule 1: SHIGA-LIKE TOXIN IIE B SUBUNIT

Chain P:  % 84% 16%


## ● Molecule 1: SHIGA-LIKE TOXIN IIE B SUBUNIT

Chain Q:  84% 16%

## ● Molecule 1: SHIGA-LIKE TOXIN IIE B SUBUNIT

Chain R:  91% 9%

## ● Molecule 1: SHIGA-LIKE TOXIN IIE B SUBUNIT

Chain S:  90% 10%

## ● Molecule 1: SHIGA-LIKE TOXIN IIE B SUBUNIT

Chain T:  91% 9%

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.49Å 54.51Å 116.89Å 90.00° 109.12° 90.00°	Depositor
Resolution (Å)	21.00 – 2.35 20.36 – 2.35	Depositor EDS
% Data completeness (in resolution range)	60.4 (21.00-2.35) 60.5 (20.36-2.35)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.21 (at 2.35Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, $R_{free}$	0.188 , 0.234 0.188 , 0.233	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	28.9	Xtriage
Anisotropy	0.437	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 34.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.012 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11019	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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, 0.333 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	0.58	0/543	0.73	0/733
1	B	0.60	0/543	0.72	0/733
1	C	0.63	0/543	0.71	0/733
1	D	0.57	0/543	0.72	0/733
1	E	0.56	0/543	0.72	0/733
1	F	0.57	0/543	0.70	0/733
1	G	0.60	0/543	0.73	0/733
1	H	0.62	0/543	0.70	0/733
1	I	0.63	0/543	0.73	0/733
1	J	0.58	0/543	0.71	0/733
1	K	0.57	0/543	0.70	0/733
1	L	0.60	0/543	0.76	1/733 (0.1%)
1	M	0.53	0/543	0.69	0/733
1	N	0.67	0/543	0.78	0/733
1	O	0.68	0/543	0.76	0/733
1	P	0.58	0/543	0.73	0/733
1	Q	0.63	0/543	0.76	0/733
1	R	0.59	0/543	0.68	0/733
1	S	0.61	0/543	0.73	1/733 (0.1%)
1	T	0.56	0/543	0.70	0/733
All	All	0.60	0/10860	0.72	2/14660 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	435	ASN	CB-CA-C	-5.22	99.96	110.40
1	L	269	ASN	N-CA-C	5.08	124.70	111.00

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	533	0	507	13	0
1	B	533	0	507	17	0
1	C	533	0	507	16	0
1	D	533	0	507	7	0
1	E	533	0	507	9	0
1	F	533	0	507	16	0
1	G	533	0	507	11	0
1	H	533	0	507	13	0
1	I	533	0	507	9	0
1	J	533	0	507	13	0
1	K	533	0	507	13	0
1	L	533	0	507	8	0
1	M	533	0	507	11	0
1	N	533	0	507	20	0
1	O	533	0	507	33	0
1	P	533	0	507	28	0
1	Q	533	0	507	25	0
1	R	533	0	507	8	0
1	S	533	0	507	8	0
1	T	533	0	507	6	0
2	A	25	0	0	3	0
2	B	16	0	0	0	0
2	C	12	0	0	4	0
2	D	16	0	0	1	0
2	E	15	0	0	4	0
2	F	14	0	0	1	0
2	G	19	0	0	2	0
2	H	13	0	0	0	0
2	I	25	0	0	3	0
2	J	24	0	0	4	0
2	K	18	0	0	0	0
2	L	10	0	0	0	0
2	M	13	0	0	1	0
2	N	14	0	0	1	0
2	O	22	0	0	2	0
2	P	20	0	0	5	0
2	Q	17	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	19	0	0	1	0
2	S	27	0	0	5	0
2	T	20	0	0	0	0
All	All	11019	0	10140	201	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 10.

All (201) 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:P:156:THR:HB	2:P:2017:HOH:O	1.46	1.13
1:N:439:LEU:HB3	1:O:541:GLN:HE22	1.10	1.09
1:O:533:ARG:NH1	1:O:564:ALA:HB1	1.69	1.08
1:P:139:LEU:HB3	1:Q:241:GLN:HE22	1.17	1.08
1:F:118:ASN:HB3	1:F:134:TRP:CH2	1.92	1.04
1:N:439:LEU:HB3	1:O:541:GLN:NE2	1.74	1.01
1:R:318:ASN:HB3	1:R:334:TRP:CH2	1.97	1.00
1:N:435:ASN:ND2	1:O:534:TRP:CH2	2.28	0.99
1:B:239:LEU:HD21	2:C:2008:HOH:O	1.63	0.98
1:I:408:LYS:HE3	2:I:2003:HOH:O	1.65	0.95
1:P:135:ASN:ND2	1:Q:234:TRP:CH2	2.34	0.95
1:K:145:LEU:HD21	1:O:546:THR:HG21	1.47	0.94
1:P:135:ASN:HD21	1:Q:234:TRP:HH2	1.12	0.93
1:P:139:LEU:HB3	1:Q:241:GLN:NE2	1.85	0.91
1:F:134:TRP:HD1	2:N:2002:HOH:O	1.53	0.90
1:O:533:ARG:HH11	1:O:533:ARG:HG3	1.36	0.89
1:N:439:LEU:HD22	1:O:541:GLN:CD	1.93	0.89
2:J:2001:HOH:O	1:L:234:TRP:HB3	1.74	0.88
1:P:139:LEU:HD22	1:Q:241:GLN:CD	1.97	0.85
1:A:158:SER:HB3	2:A:2021:HOH:O	1.79	0.82
1:F:118:ASN:HB3	1:F:134:TRP:CZ2	2.16	0.81
1:N:435:ASN:HD21	1:O:534:TRP:HH2	1.23	0.81
1:A:118:ASN:HB3	2:A:2005:HOH:O	1.80	0.80
1:O:533:ARG:HH12	1:O:564:ALA:HB1	1.44	0.80
1:H:325:SER:CA	1:Q:256:THR:HG21	2.12	0.79
1:H:325:SER:HA	1:Q:256:THR:HG21	1.65	0.78
1:O:514:TYR:HD2	2:O:2010:HOH:O	1.67	0.77
1:N:439:LEU:CB	1:O:541:GLN:HE22	1.95	0.77
1:K:145:LEU:HD21	1:O:546:THR:CG2	2.14	0.76
1:O:537:GLN:HG3	2:O:2011:HOH:O	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ASN:HA	1:E:565:GLU:HG3	1.70	0.73
1:L:248:MET:SD	1:M:345:LEU:HD21	2.29	0.72
1:N:439:LEU:CD2	1:O:541:GLN:OE1	2.37	0.72
1:P:139:LEU:CD2	1:Q:241:GLN:OE1	2.39	0.71
1:L:248:MET:SD	1:M:345:LEU:CD2	2.78	0.71
1:A:110:GLU:HG3	2:A:2003:HOH:O	1.89	0.71
1:E:518:ASN:HA	2:E:2007:HOH:O	1.91	0.70
1:P:139:LEU:CB	1:Q:241:GLN:HE22	2.00	0.69
1:N:439:LEU:HD22	1:O:541:GLN:OE1	1.92	0.69
1:S:433:ARG:NE	2:S:2012:HOH:O	2.24	0.67
1:A:134:TRP:CE3	2:P:2005:HOH:O	2.47	0.67
1:P:139:LEU:HA	1:Q:241:GLN:OE1	1.94	0.66
1:I:435:ASN:HD21	1:M:334:TRP:HZ2	1.41	0.66
1:P:139:LEU:HD22	1:Q:241:GLN:OE1	1.95	0.66
1:M:365:GLU:HG3	1:N:415:ASN:HA	1.78	0.65
1:H:325:SER:CB	1:Q:256:THR:HG21	2.28	0.64
1:J:555:ASN:OD1	1:K:118:ASN:ND2	2.31	0.64
1:F:118:ASN:CB	1:F:134:TRP:CH2	2.77	0.64
1:F:134:TRP:HB2	2:F:2007:HOH:O	1.96	0.64
1:D:434:TRP:CZ2	1:T:532:ASN:HB2	2.34	0.63
1:N:439:LEU:HA	1:O:541:GLN:OE1	1.99	0.63
1:O:533:ARG:HG3	1:O:533:ARG:NH1	2.06	0.63
1:K:146:THR:HG21	1:L:245:LEU:HD13	1.82	0.62
1:F:115:ASN:HA	1:J:565:GLU:HG3	1.83	0.61
1:K:145:LEU:HD21	1:O:546:THR:CB	2.31	0.61
1:K:145:LEU:HD11	1:O:546:THR:HB	1.83	0.60
1:A:133:ARG:NE	1:P:132:ASN:HD21	2.01	0.58
1:F:118:ASN:HB3	1:F:134:TRP:HH2	1.62	0.57
1:J:556:THR:HB	2:J:2021:HOH:O	2.03	0.57
1:G:231:THR:HA	2:G:2010:HOH:O	2.05	0.56
1:I:416:GLU:HG3	2:I:2005:HOH:O	2.06	0.56
1:F:117:ASP:O	1:F:118:ASN:HB2	2.05	0.56
1:M:336:LEU:HD21	1:N:414:TYR:CG	2.40	0.56
1:O:533:ARG:HH11	1:O:564:ALA:HB1	1.67	0.56
1:P:114:TYR:CG	1:T:536:LEU:HD21	2.41	0.56
1:H:318:ASN:HB3	1:H:334:TRP:CH2	2.41	0.55
1:R:318:ASN:HB3	1:R:334:TRP:HH2	1.65	0.55
1:L:265:GLU:HG3	1:M:315:ASN:HA	1.89	0.55
1:P:139:LEU:HD21	2:Q:2007:HOH:O	2.05	0.55
1:I:465:GLU:HG3	1:J:515:ASN:HA	1.88	0.54
1:A:133:ARG:HD3	1:P:132:ASN:ND2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:ARG:NH1	1:C:314:TYR:HE1	2.06	0.54
1:P:139:LEU:HD23	1:Q:241:GLN:OE1	2.08	0.53
1:Q:217:ASP:O	1:Q:218:ASN:HB2	2.09	0.53
1:S:408:LYS:HG2	2:S:2007:HOH:O	2.09	0.53
1:N:439:LEU:CB	1:O:541:GLN:NE2	2.59	0.53
1:N:465:GLU:HG3	1:O:514:TYR:O	2.08	0.53
1:B:218:ASN:ND2	1:P:130:TRP:CH2	2.77	0.52
1:C:369:ASN:HA	2:C:2012:HOH:O	2.08	0.52
1:G:235:ASN:O	1:G:238:PRO:HD2	2.09	0.52
1:N:439:LEU:HD23	1:O:541:GLN:OE1	2.09	0.52
1:P:165:GLU:HG3	1:Q:214:TYR:O	2.10	0.52
1:Q:241:GLN:HG2	1:Q:245:LEU:HG	1.92	0.52
1:F:118:ASN:CB	1:F:134:TRP:HH2	2.21	0.51
1:J:517:ASP:O	1:J:518:ASN:HB2	2.10	0.51
1:P:139:LEU:CB	1:Q:241:GLN:NE2	2.66	0.51
1:Q:211:PHE:CD1	1:Q:211:PHE:C	2.84	0.51
1:M:341:GLN:O	1:M:345:LEU:HG	2.11	0.50
1:B:218:ASN:ND2	1:P:130:TRP:CZ3	2.79	0.50
1:E:517:ASP:O	1:E:518:ASN:HB2	2.11	0.50
1:F:134:TRP:CE3	1:J:535:ASN:ND2	2.80	0.50
1:G:208:LYS:HD2	1:G:247:GLY:O	2.12	0.50
1:R:318:ASN:CB	1:R:334:TRP:CH2	2.83	0.50
1:Q:267:GLN:HE21	1:Q:269:ASN:HD21	1.58	0.50
1:C:311:PHE:CD1	1:C:311:PHE:C	2.84	0.50
1:H:318:ASN:ND2	1:M:355:ASN:OD1	2.45	0.49
1:C:311:PHE:CE2	1:C:323:LYS:HD2	2.47	0.49
1:C:317:ASP:O	1:C:318:ASN:HB2	2.13	0.49
1:B:239:LEU:CD2	1:C:341:GLN:OE1	2.61	0.49
1:B:239:LEU:CD2	2:C:2008:HOH:O	2.40	0.49
1:P:115:ASN:HA	1:T:565:GLU:HG3	1.95	0.48
1:F:118:ASN:OD1	1:J:533:ARG:NH1	2.46	0.48
1:J:534:TRP:HB3	2:J:2008:HOH:O	2.13	0.48
1:R:365:GLU:HG3	1:S:415:ASN:HA	1.95	0.47
1:E:518:ASN:CA	2:E:2007:HOH:O	2.56	0.47
1:P:132:ASN:CB	2:P:2009:HOH:O	2.62	0.47
1:B:239:LEU:HD11	2:C:2008:HOH:O	2.13	0.47
1:K:145:LEU:HD21	1:O:546:THR:OG1	2.14	0.47
1:A:132:ASN:HB2	1:P:133:ARG:HH11	1.79	0.47
1:B:239:LEU:HD22	1:C:341:GLN:CD	2.35	0.47
1:F:111:PHE:C	1:F:111:PHE:CD1	2.88	0.47
1:B:265:GLU:HG3	1:C:315:ASN:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:511:PHE:C	1:J:511:PHE:CD1	2.88	0.47
1:T:511:PHE:CE2	1:T:523:LYS:HD2	2.50	0.47
1:P:135:ASN:ND2	1:Q:234:TRP:HH2	1.92	0.47
1:G:211:PHE:CD1	1:G:211:PHE:C	2.89	0.46
1:Q:234:TRP:HA	1:Q:234:TRP:CE3	2.50	0.46
1:A:136:LEU:HD21	1:B:214:TYR:CG	2.50	0.46
1:H:325:SER:HB3	1:Q:256:THR:HG21	1.97	0.46
1:I:411:PHE:C	1:I:411:PHE:CD1	2.88	0.46
1:L:211:PHE:C	1:L:211:PHE:CD1	2.89	0.46
1:D:465:GLU:HG3	1:E:515:ASN:HA	1.96	0.46
1:O:511:PHE:C	1:O:511:PHE:CD1	2.88	0.46
1:G:210:GLU:OE1	2:G:2006:HOH:O	2.20	0.46
1:P:111:PHE:CD1	1:P:111:PHE:C	2.89	0.46
1:O:517:ASP:O	1:O:518:ASN:HB2	2.16	0.46
1:N:433:ARG:NE	1:O:514:TYR:OH	2.49	0.46
1:R:317:ASP:O	1:R:318:ASN:HB2	2.16	0.46
1:F:118:ASN:CG	1:F:134:TRP:HH2	2.18	0.45
1:G:246:THR:HG21	1:H:345:LEU:HD22	1.98	0.45
1:E:501:ALA:CA	2:E:2004:HOH:O	2.64	0.45
1:K:165:GLU:HG3	1:L:215:ASN:HA	1.98	0.45
1:S:411:PHE:C	1:S:411:PHE:CD1	2.90	0.45
1:H:311:PHE:C	1:H:311:PHE:CD1	2.89	0.45
1:S:448:MET:O	2:S:2020:HOH:O	2.21	0.45
1:G:265:GLU:HG3	1:H:315:ASN:HA	1.97	0.45
1:D:417:ASP:O	1:D:418:ASN:HB2	2.17	0.45
1:A:133:ARG:CD	1:P:132:ASN:ND2	2.80	0.45
1:C:346:THR:OG1	1:D:445:LEU:HD21	2.15	0.45
1:E:511:PHE:CD1	1:E:511:PHE:C	2.91	0.45
1:K:111:PHE:CD1	1:K:111:PHE:C	2.91	0.44
1:P:139:LEU:HD11	2:Q:2007:HOH:O	2.17	0.44
1:F:165:GLU:HG3	1:G:215:ASN:HA	1.98	0.44
1:B:233:ARG:HH11	1:C:314:TYR:HE1	1.65	0.44
1:F:133:ARG:CZ	1:F:164:ALA:HB1	2.47	0.44
1:D:411:PHE:CD1	1:D:411:PHE:C	2.90	0.44
1:S:433:ARG:NH2	2:S:2012:HOH:O	2.50	0.44
1:N:411:PHE:C	1:N:411:PHE:CD1	2.90	0.44
1:N:439:LEU:CD2	1:O:541:GLN:CD	2.73	0.44
1:M:311:PHE:CD1	1:M:311:PHE:C	2.90	0.44
1:G:217:ASP:O	1:G:218:ASN:HB2	2.18	0.43
1:D:433:ARG:NE	2:D:2007:HOH:O	2.36	0.43
1:O:533:ARG:HH12	1:O:564:ALA:CB	2.24	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:511:PHE:CE2	1:J:523:LYS:HD2	2.54	0.43
1:B:211:PHE:CD1	1:B:211:PHE:C	2.92	0.43
1:C:349:THR:HB	1:C:369:ASN:HB2	2.00	0.43
1:C:312:SER:HB2	1:C:320:PHE:CZ	2.53	0.43
1:K:145:LEU:CD2	1:O:546:THR:HG21	2.33	0.43
1:T:511:PHE:C	1:T:511:PHE:CD1	2.91	0.43
1:N:418:ASN:HB3	1:N:434:TRP:CH2	2.54	0.43
1:R:311:PHE:C	1:R:311:PHE:CD1	2.92	0.42
1:H:318:ASN:HB3	1:H:334:TRP:CZ3	2.54	0.42
1:A:111:PHE:C	1:A:111:PHE:CD1	2.93	0.42
1:B:239:LEU:HD23	1:C:341:GLN:OE1	2.20	0.42
1:E:501:ALA:C	2:E:2004:HOH:O	2.57	0.42
1:B:239:LEU:HD22	1:C:341:GLN:OE1	2.19	0.42
1:J:518:ASN:HA	2:J:2007:HOH:O	2.19	0.42
1:O:533:ARG:CG	1:O:533:ARG:NH1	2.75	0.42
1:S:433:ARG:CZ	2:S:2012:HOH:O	2.65	0.42
1:E:532:ASN:HB2	1:S:434:TRP:CZ2	2.55	0.42
1:A:156:THR:HG22	1:I:428:GLU:CD	2.40	0.42
1:B:265:GLU:HG3	1:C:314:TYR:O	2.20	0.42
1:D:467:GLN:HE21	1:D:469:ASN:HD21	1.68	0.42
1:I:416:GLU:CG	2:I:2005:HOH:O	2.65	0.42
1:K:117:ASP:O	1:K:118:ASN:HB2	2.20	0.42
1:B:211:PHE:HA	1:B:244:GLN:NE2	2.35	0.42
1:N:435:ASN:ND2	1:O:534:TRP:HH2	1.94	0.42
1:Q:267:GLN:HE21	1:Q:269:ASN:ND2	2.18	0.42
1:C:320:PHE:O	1:C:330:TRP:HA	2.20	0.41
1:H:317:ASP:O	1:H:318:ASN:HB2	2.20	0.41
1:O:548:MET:HE2	1:O:568:PHE:HB3	2.02	0.41
1:P:101:ALA:N	2:P:2001:HOH:O	2.53	0.41
1:F:136:LEU:HD21	1:G:214:TYR:CG	2.55	0.41
1:H:325:SER:HA	1:Q:256:THR:CG2	2.43	0.41
1:M:311:PHE:CE2	1:M:323:LYS:HD2	2.55	0.41
1:J:536:LEU:HD23	1:J:536:LEU:HA	1.93	0.41
1:K:136:LEU:HD21	1:L:214:TYR:CG	2.56	0.41
1:B:236:LEU:HD23	1:B:239:LEU:HD12	2.03	0.41
1:H:365:GLU:HG3	1:I:415:ASN:HA	2.02	0.41
1:R:308:LYS:HE2	2:R:2017:HOH:O	2.20	0.41
1:M:317:ASP:O	1:M:318:ASN:HB2	2.21	0.41
1:R:318:ASN:CB	1:R:334:TRP:HH2	2.30	0.40
1:J:534:TRP:CH2	2:M:2008:HOH:O	2.72	0.40
1:K:136:LEU:HA	1:K:136:LEU:HD23	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:132:ASN:HB2	2:P:2009:HOH:O	2.20	0.40
1:Q:267:GLN:NE2	1:Q:269:ASN:HD21	2.18	0.40
1:I:412:SER:HA	1:I:421:THR:O	2.20	0.40
1:N:418:ASN:O	1:N:434:TRP:HZ3	2.04	0.40
1:T:545:LEU:HD23	1:T:545:LEU:HA	1.87	0.40
1:A:133:ARG:HB2	1:A:136:LEU:HD12	2.04	0.40
1:G:242:SER:HA	1:G:245:LEU:HD12	2.03	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	66/68 (97%)	65 (98%)	1 (2%)	0	100	100
1	B	66/68 (97%)	66 (100%)	0	0	100	100
1	C	66/68 (97%)	64 (97%)	2 (3%)	0	100	100
1	D	66/68 (97%)	65 (98%)	1 (2%)	0	100	100
1	E	66/68 (97%)	65 (98%)	1 (2%)	0	100	100
1	F	66/68 (97%)	66 (100%)	0	0	100	100
1	G	66/68 (97%)	65 (98%)	1 (2%)	0	100	100
1	H	66/68 (97%)	65 (98%)	1 (2%)	0	100	100
1	I	66/68 (97%)	65 (98%)	1 (2%)	0	100	100
1	J	66/68 (97%)	65 (98%)	1 (2%)	0	100	100
1	K	66/68 (97%)	64 (97%)	2 (3%)	0	100	100
1	L	66/68 (97%)	64 (97%)	2 (3%)	0	100	100
1	M	66/68 (97%)	64 (97%)	2 (3%)	0	100	100
1	N	66/68 (97%)	66 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	66/68 (97%)	64 (97%)	2 (3%)	0	100	100
1	P	66/68 (97%)	66 (100%)	0	0	100	100
1	Q	66/68 (97%)	63 (96%)	3 (4%)	0	100	100
1	R	66/68 (97%)	66 (100%)	0	0	100	100
1	S	66/68 (97%)	65 (98%)	1 (2%)	0	100	100
1	T	66/68 (97%)	65 (98%)	1 (2%)	0	100	100
All	All	1320/1360 (97%)	1298 (98%)	22 (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	59/59 (100%)	58 (98%)	1 (2%)	66	77
1	B	59/59 (100%)	59 (100%)	0	100	100
1	C	59/59 (100%)	57 (97%)	2 (3%)	42	53
1	D	59/59 (100%)	59 (100%)	0	100	100
1	E	59/59 (100%)	59 (100%)	0	100	100
1	F	59/59 (100%)	59 (100%)	0	100	100
1	G	59/59 (100%)	58 (98%)	1 (2%)	66	77
1	H	59/59 (100%)	59 (100%)	0	100	100
1	I	59/59 (100%)	59 (100%)	0	100	100
1	J	59/59 (100%)	59 (100%)	0	100	100
1	K	59/59 (100%)	59 (100%)	0	100	100
1	L	59/59 (100%)	58 (98%)	1 (2%)	66	77
1	M	59/59 (100%)	59 (100%)	0	100	100
1	N	59/59 (100%)	58 (98%)	1 (2%)	66	77
1	O	59/59 (100%)	59 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	59/59 (100%)	59 (100%)	0	100	100
1	Q	59/59 (100%)	58 (98%)	1 (2%)	66	77
1	R	59/59 (100%)	59 (100%)	0	100	100
1	S	59/59 (100%)	59 (100%)	0	100	100
1	T	59/59 (100%)	59 (100%)	0	100	100
All	All	1180/1180 (100%)	1173 (99%)	7 (1%)	89	94

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	TRP
1	C	311	PHE
1	C	335	ASN
1	G	246	THR
1	L	250	VAL
1	N	434	TRP
1	Q	235	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	ASN
1	A	167	GLN
1	B	255	ASN
1	B	269	ASN
1	C	355	ASN
1	D	455	ASN
1	D	467	GLN
1	E	518	ASN
1	E	555	ASN
1	E	567	GLN
1	E	569	ASN
1	F	155	ASN
1	F	167	GLN
1	F	169	ASN
1	G	255	ASN
1	H	355	ASN
1	H	367	GLN
1	I	455	ASN

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Mol	Chain	Res	Type
1	J	555	ASN
1	K	118	ASN
1	K	155	ASN
1	K	167	GLN
1	K	169	ASN
1	L	255	ASN
1	N	455	ASN
1	O	555	ASN
1	O	567	GLN
1	O	569	ASN
1	P	132	ASN
1	P	155	ASN
1	P	169	ASN
1	Q	255	ASN
1	Q	267	GLN
1	R	355	ASN
1	S	455	ASN
1	S	467	GLN
1	T	518	ASN

### 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<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	68/68 (100%)	-0.38	0 100 100	15, 26, 37, 46	0
1	B	68/68 (100%)	-0.39	1 (1%) 74 83	17, 27, 42, 50	0
1	C	68/68 (100%)	-0.09	2 (2%) 52 63	19, 30, 44, 58	0
1	D	68/68 (100%)	-0.44	0 100 100	16, 28, 41, 48	0
1	E	68/68 (100%)	-0.40	0 100 100	16, 27, 41, 50	0
1	F	68/68 (100%)	-0.29	1 (1%) 74 83	16, 26, 44, 56	0
1	G	68/68 (100%)	-0.33	0 100 100	18, 29, 40, 49	0
1	H	68/68 (100%)	-0.25	1 (1%) 74 83	17, 27, 43, 56	0
1	I	68/68 (100%)	-0.37	0 100 100	12, 25, 39, 49	0
1	J	68/68 (100%)	-0.42	0 100 100	16, 26, 41, 50	0
1	K	68/68 (100%)	-0.40	2 (2%) 52 63	17, 26, 41, 52	0
1	L	68/68 (100%)	-0.33	0 100 100	17, 27, 43, 52	0
1	M	68/68 (100%)	-0.33	1 (1%) 74 83	18, 28, 43, 49	0
1	N	68/68 (100%)	-0.32	0 100 100	16, 28, 42, 50	0
1	O	68/68 (100%)	-0.18	0 100 100	17, 27, 39, 50	0
1	P	68/68 (100%)	-0.31	1 (1%) 74 83	18, 28, 43, 50	0
1	Q	68/68 (100%)	-0.16	0 100 100	17, 28, 42, 50	0
1	R	68/68 (100%)	-0.46	0 100 100	15, 27, 41, 50	0
1	S	68/68 (100%)	-0.37	0 100 100	17, 26, 39, 47	0
1	T	68/68 (100%)	-0.47	0 100 100	16, 28, 42, 49	0
All	All	1360/1360 (100%)	-0.33	9 (0%) 87 93	12, 27, 43, 58	0

All (9) RSRZ outliers are listed below:



Mol	Chain	Res	Type	RSRZ
1	F	134	TRP	3.4
1	C	334	TRP	3.0
1	K	134	TRP	2.8
1	H	334	TRP	2.6
1	P	164	ALA	2.3
1	K	156	THR	2.3
1	M	358	SER	2.2
1	C	355	ASN	2.1
1	B	258	SER	2.1

## 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.