Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:06 PM GMT

PDB ID	:	1ILU
Title	:	X-RAY CRYSTAL STRUCTURE THE TWO SITE-SPECIFIC MUTANTS ILE7SER AND PHE110SER OF AZURIN FROM PSEUDOMONAS AERUGINOSA
Authors	:	Hammann, C.; Nar, H.; Huber, R.; Messerschmidt, A.
Deposited on	:	1995-10-12
Resolution	:	2.30 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

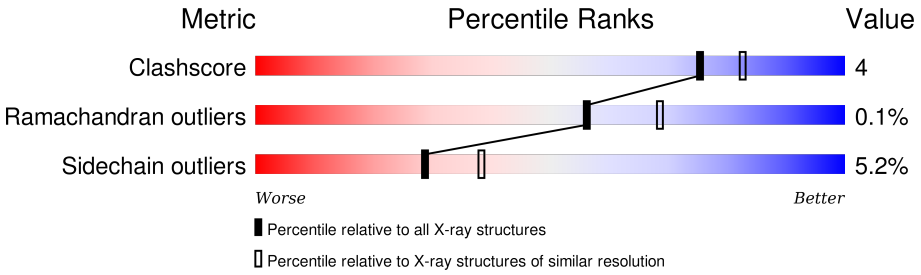
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.30 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))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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 >=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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	128	85% 13% •
1	B	128	88% 13%
1	C	128	88% 10% •
1	D	128	79% 20% ••
1	E	128	88% 11% •
1	F	128	84% 16% •
1	G	128	84% 14% •

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Mol	Chain	Length	Quality of chain
1	H	128	
1	I	128	
1	K	128	
1	L	128	
1	M	128	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16428 atoms, of which 4072 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 AZURIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			
1	B	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			
1	C	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			
1	D	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			
1	E	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			
1	F	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			
1	G	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			
1	H	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			
1	I	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			
1	K	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			
1	L	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			
1	M	128	Total	C	H	N	O	S	0	0	0
			1189	601	220	164	195	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	SER	PHE	ENGINEERED	UNP P00282
B	110	SER	PHE	ENGINEERED	UNP P00282
C	110	SER	PHE	ENGINEERED	UNP P00282
D	110	SER	PHE	ENGINEERED	UNP P00282
E	110	SER	PHE	ENGINEERED	UNP P00282

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Chain	Residue	Modelled	Actual	Comment	Reference
F	110	SER	PHE	ENGINEERED	UNP P00282
G	110	SER	PHE	ENGINEERED	UNP P00282
H	110	SER	PHE	ENGINEERED	UNP P00282
I	110	SER	PHE	ENGINEERED	UNP P00282
K	110	SER	PHE	ENGINEERED	UNP P00282
L	110	SER	PHE	ENGINEERED	UNP P00282
M	110	SER	PHE	ENGINEERED	UNP P00282

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Cu 1 1	0	0
2	D	1	Total Cu 1 1	0	0
2	K	1	Total Cu 1 1	0	0
2	E	1	Total Cu 1 1	0	0
2	H	1	Total Cu 1 1	0	0
2	B	1	Total Cu 1 1	0	0
2	I	1	Total Cu 1 1	0	0
2	C	1	Total Cu 1 1	0	0
2	A	1	Total Cu 1 1	0	0
2	L	1	Total Cu 1 1	0	0
2	F	1	Total Cu 1 1	0	0
2	M	1	Total Cu 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	63	Total H O 189 126 63	0	0
3	B	83	Total H O 249 166 83	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	63	Total H O 189 126 63	0	0
3	D	55	Total H O 165 110 55	0	0
3	E	61	Total H O 183 122 61	0	0
3	F	47	Total H O 141 94 47	0	0
3	G	54	Total H O 162 108 54	0	0
3	H	55	Total H O 165 110 55	0	0
3	I	52	Total H O 156 104 52	0	0
3	K	62	Total H O 186 124 62	0	0
3	L	62	Total H O 186 124 62	0	0
3	M	59	Total H O 177 118 59	0	0

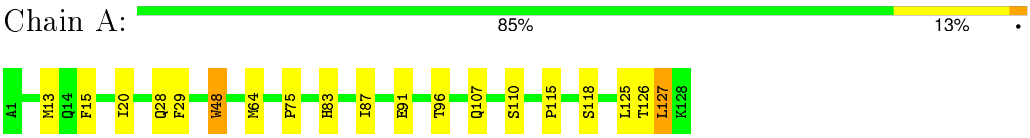
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

Note EDS was not executed.

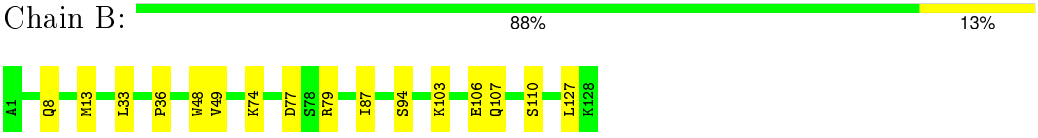
- Molecule 1: AZURIN

Chain A:



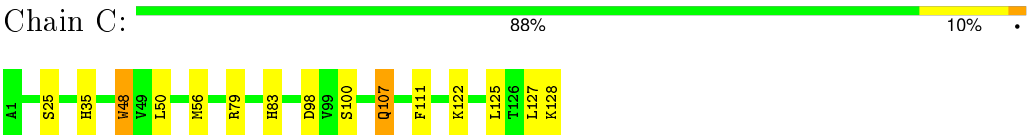
- Molecule 1: AZURIN

Chain B:



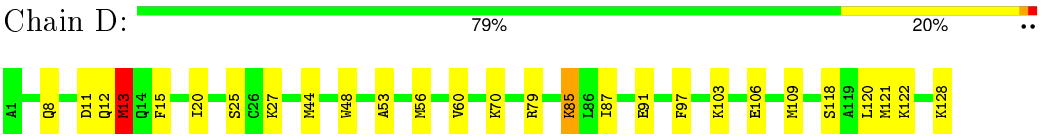
- Molecule 1: AZURIN

Chain C:



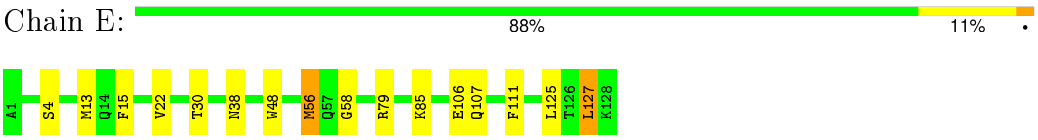
- Molecule 1: AZURIN

Chain D:



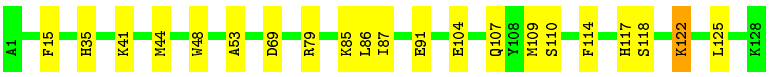
- Molecule 1: AZURIN

Chain E:



- Molecule 1: AZURIN

Chain F:

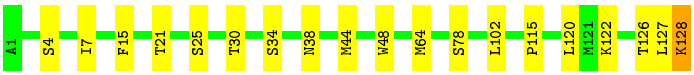


• Molecule 1: AZURIN

Chain G:

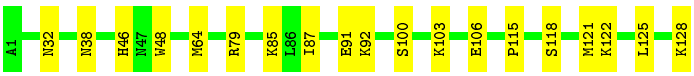
• Molecule 1: AZURIN

Chain H:



• Molecule 1: AZURIN

Chain I:

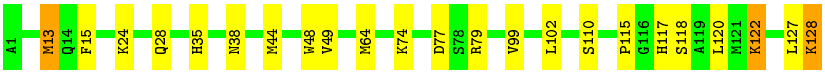


• Molecule 1: AZURIN

Chain K:

• Molecule 1: AZURIN

Chain L:



• Molecule 1: AZURIN

Chain M:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	41.40Å 170.10Å 99.70Å 90.00° 91.30° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.30)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.171 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16428	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU

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	0.73	1/985 (0.1%)	1.38	7/1327 (0.5%)
1	B	0.69	0/985	1.35	9/1327 (0.7%)
1	C	0.71	0/985	1.28	5/1327 (0.4%)
1	D	0.68	0/985	1.31	6/1327 (0.5%)
1	E	0.70	0/985	1.34	7/1327 (0.5%)
1	F	0.68	0/985	1.33	9/1327 (0.7%)
1	G	0.71	0/985	1.38	8/1327 (0.6%)
1	H	0.71	0/985	1.29	6/1327 (0.5%)
1	I	0.70	0/985	1.34	8/1327 (0.6%)
1	K	0.68	0/985	1.30	5/1327 (0.4%)
1	L	0.70	0/985	1.34	10/1327 (0.8%)
1	M	0.70	0/985	1.32	6/1327 (0.5%)
All	All	0.70	1/11820 (0.0%)	1.33	86/15924 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	107	GLN	CB-CG	-5.78	1.36	1.52

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	48	TRP	CD1-CG-CD2	9.40	113.82	106.30
1	E	56	MET	CG-SD-CE	-9.31	85.30	100.20
1	A	48	TRP	CD1-CG-CD2	8.96	113.46	106.30
1	I	79	ARG	NE-CZ-NH1	8.83	124.71	120.30
1	H	48	TRP	CD1-CG-CD2	8.72	113.28	106.30
1	B	48	TRP	CD1-CG-CD2	8.58	113.17	106.30
1	F	48	TRP	CE2-CD2-CG	-8.56	100.45	107.30
1	C	48	TRP	CD1-CG-CD2	8.48	113.09	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	48	TRP	CD1-CG-CD2	8.42	113.03	106.30
1	I	48	TRP	CD1-CG-CD2	8.23	112.88	106.30
1	M	48	TRP	CE2-CD2-CG	-8.13	100.80	107.30
1	G	48	TRP	CE2-CD2-CG	-8.07	100.84	107.30
1	A	48	TRP	CE2-CD2-CG	-8.04	100.87	107.30
1	G	48	TRP	CD1-CG-CD2	7.98	112.69	106.30
1	H	48	TRP	CE2-CD2-CG	-7.79	101.07	107.30
1	B	48	TRP	CE2-CD2-CG	-7.75	101.10	107.30
1	I	48	TRP	CE2-CD2-CG	-7.63	101.20	107.30
1	C	48	TRP	CE2-CD2-CG	-7.62	101.21	107.30
1	E	48	TRP	CE2-CD2-CG	-7.58	101.23	107.30
1	L	48	TRP	CE2-CD2-CG	-7.54	101.27	107.30
1	M	48	TRP	CD1-CG-CD2	7.51	112.31	106.30
1	D	48	TRP	CE2-CD2-CG	-7.48	101.31	107.30
1	B	79	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	E	48	TRP	CD1-CG-CD2	7.43	112.24	106.30
1	D	48	TRP	CD1-CG-CD2	7.38	112.20	106.30
1	K	48	TRP	CD1-CG-CD2	7.30	112.14	106.30
1	K	48	TRP	CE2-CD2-CG	-7.29	101.47	107.30
1	M	13	MET	CA-CB-CG	7.24	125.61	113.30
1	A	13	MET	CA-CB-CG	7.07	125.32	113.30
1	L	79	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	B	13	MET	CA-CB-CG	6.80	124.85	113.30
1	I	79	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	G	79	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	M	48	TRP	CG-CD2-CE3	6.44	139.70	133.90
1	I	122	LYS	CB-CA-C	-6.28	97.83	110.40
1	E	79	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	E	13	MET	CA-CB-CG	6.26	123.94	113.30
1	D	13	MET	CA-CB-CG	6.25	123.92	113.30
1	G	59	VAL	CG1-CB-CG2	-6.25	100.90	110.90
1	G	48	TRP	CG-CD2-CE3	6.24	139.52	133.90
1	F	48	TRP	CG-CD2-CE3	6.23	139.50	133.90
1	B	79	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	A	127	LEU	CA-CB-CG	6.17	129.48	115.30
1	K	13	MET	CA-CB-CG	6.16	123.76	113.30
1	L	128	LYS	CA-CB-CG	6.13	126.88	113.40
1	B	48	TRP	CG-CD2-CE3	6.09	139.38	133.90
1	F	44	MET	CA-CB-CG	6.07	123.62	113.30
1	D	48	TRP	CB-CG-CD1	-6.05	119.13	127.00
1	G	48	TRP	CB-CG-CD1	-6.05	119.14	127.00
1	K	79	ARG	NE-CZ-NH2	-6.02	117.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	108	TYR	CB-CG-CD2	-5.95	117.43	121.00
1	F	122	LYS	CA-CB-CG	5.92	126.43	113.40
1	B	48	TRP	CB-CG-CD1	-5.83	119.42	127.00
1	A	48	TRP	CB-CG-CD1	-5.82	119.43	127.00
1	I	48	TRP	CB-CG-CD1	-5.76	119.50	127.00
1	F	48	TRP	CG-CD1-NE1	-5.67	104.44	110.10
1	H	48	TRP	CG-CD1-NE1	-5.66	104.44	110.10
1	H	48	TRP	CB-CG-CD1	-5.62	119.69	127.00
1	M	48	TRP	CB-CG-CD1	-5.62	119.69	127.00
1	A	48	TRP	CG-CD1-NE1	-5.61	104.49	110.10
1	L	122	LYS	CA-CB-CG	5.58	125.68	113.40
1	L	48	TRP	CB-CG-CD1	-5.54	119.80	127.00
1	I	48	TRP	CG-CD2-CE3	5.53	138.88	133.90
1	G	12	GLN	CA-CB-CG	5.51	125.52	113.40
1	L	127	LEU	CA-CB-CG	5.50	127.95	115.30
1	H	44	MET	CA-CB-CG	5.50	122.65	113.30
1	F	48	TRP	CB-CG-CD1	-5.46	119.90	127.00
1	A	48	TRP	CG-CD2-CE3	5.43	138.79	133.90
1	E	48	TRP	CG-CD2-CE3	5.43	138.79	133.90
1	C	48	TRP	CB-CG-CD1	-5.42	119.96	127.00
1	C	48	TRP	CG-CD1-NE1	-5.38	104.72	110.10
1	D	48	TRP	CG-CD2-CE3	5.37	138.73	133.90
1	D	79	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	C	48	TRP	CG-CD2-CE3	5.34	138.71	133.90
1	L	13	MET	CG-SD-CE	-5.28	91.75	100.20
1	K	48	TRP	CB-CG-CD1	-5.27	120.15	127.00
1	B	48	TRP	CG-CD1-NE1	-5.26	104.84	110.10
1	E	48	TRP	CB-CG-CD1	-5.24	120.18	127.00
1	M	14	GLN	CA-CB-CG	5.22	124.89	113.40
1	F	79	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	I	48	TRP	CG-CD1-NE1	-5.17	104.93	110.10
1	H	48	TRP	CG-CD2-CE3	5.11	138.50	133.90
1	B	127	LEU	CA-CB-CG	5.09	127.02	115.30
1	F	110	SER	N-CA-CB	-5.03	102.95	110.50
1	L	48	TRP	CG-CD2-CE3	5.01	138.41	133.90
1	L	48	TRP	CG-CD1-NE1	-5.00	105.10	110.10

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	969	220	949	7	0
1	B	969	220	948	7	0
1	C	969	220	948	4	1
1	D	969	220	948	12	1
1	E	969	220	948	5	0
1	F	969	220	948	5	0
1	G	969	220	948	7	1
1	H	969	220	948	8	0
1	I	969	220	948	5	1
1	K	969	220	948	14	0
1	L	969	220	948	9	0
1	M	969	220	948	6	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
3	A	63	126	0	1	0
3	B	83	166	0	2	0
3	C	63	126	0	1	0
3	D	55	110	0	4	1
3	E	61	122	0	2	0
3	F	47	94	0	1	0
3	G	54	108	0	3	0
3	H	55	110	0	2	0
3	I	52	104	0	0	0
3	K	62	124	0	2	1
3	L	62	124	0	2	0
3	M	59	118	0	1	0
All	All	12356	4072	11377	89	3

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 4.

All (89) 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:I:32:ASN:HB3	1:I:92:LYS:HZ2	1.58	0.67
1:G:87:ILE:HB	1:G:91:GLU:HB2	1.81	0.63
1:M:34:SER:HB3	1:M:92:LYS:HD2	1.79	0.63
1:I:32:ASN:HB3	1:I:92:LYS:NZ	2.14	0.62
1:L:13:MET:HE3	1:L:117:HIS:HA	1.82	0.62
1:B:33:LEU:HD13	3:B:3007:HOH:O	2.00	0.61
1:D:13:MET:HG3	1:D:120:LEU:HD12	1.82	0.61
1:I:64:MET:HG3	1:I:115:PRO:HG3	1.83	0.60
1:A:64:MET:HG3	1:A:115:PRO:HB3	1.84	0.60
1:A:20:ILE:HB	1:A:125:LEU:HD12	1.85	0.59
1:H:21:THR:HG22	1:H:128:LYS:HG2	1.84	0.58
1:B:8:GLN:HE21	1:B:36:PRO:HG2	1.70	0.57
1:C:56:MET:HG3	1:C:111:PHE:CE1	2.41	0.55
1:F:41:LYS:HD3	1:F:86:LEU:HD23	1.89	0.55
1:D:20:ILE:HD11	3:D:1911:HOH:O	2.07	0.55
1:H:7:ILE:HB	3:H:2554:HOH:O	2.09	0.53
1:D:118:SER:HB3	3:D:570:HOH:O	2.09	0.52
1:L:13:MET:HE2	1:L:120:LEU:HD12	1.92	0.52
1:K:56:MET:O	1:K:60:VAL:HG23	2.10	0.52
1:M:23:ASP:HA	1:M:128:LYS:HB3	1.90	0.52
1:A:87:ILE:HB	1:A:91:GLU:HB2	1.92	0.52
1:M:13:MET:HE2	1:M:120:LEU:HD23	1.91	0.51
1:D:60:VAL:HG22	3:D:570:HOH:O	2.10	0.51
1:G:18:ASN:HB3	3:G:3103:HOH:O	2.08	0.51
1:K:33:LEU:O	1:K:92:LYS:HD2	2.10	0.51
1:L:99:VAL:HG13	3:L:2808:HOH:O	2.11	0.51
1:G:76:ASP:HA	3:G:3115:HOH:O	2.11	0.50
1:E:85:LYS:HB2	3:E:1542:HOH:O	2.12	0.50
1:G:29:PHE:O	1:G:96:THR:HA	2.12	0.49
1:H:102:LEU:HD12	1:H:127:LEU:HD21	1.94	0.49
1:K:87:ILE:HB	1:K:91:GLU:HB2	1.95	0.49
1:K:21:THR:HG22	1:K:126:THR:HB	1.94	0.49
1:K:13:MET:HG3	1:K:120:LEU:HD12	1.95	0.49
1:D:97:PHE:HB2	3:D:3127:HOH:O	2.13	0.48
1:B:103:LYS:HE2	1:B:106:GLU:HB2	1.95	0.48
1:L:64:MET:HG3	1:L:115:PRO:HB3	1.95	0.47
1:F:53:ALA:HA	1:F:109:MET:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:GLN:HB3	1:A:96:THR:HG22	1.96	0.47
1:B:107:GLN:HA	3:B:2926:HOH:O	2.14	0.47
1:M:16:ASN:ND2	3:M:2510:HOH:O	2.48	0.46
1:K:53:ALA:HA	1:K:109:MET:HG2	1.96	0.46
1:E:56:MET:HG3	1:E:111:PHE:CE1	2.50	0.46
1:D:56:MET:O	1:D:60:VAL:HG23	2.14	0.46
1:H:127:LEU:HD13	3:H:2645:HOH:O	2.15	0.46
1:L:24:LYS:HB2	1:L:128:LYS:OXT	2.16	0.45
1:K:104:GLU:HB2	3:K:2324:HOH:O	2.16	0.45
1:K:20:ILE:O	1:K:125:LEU:HA	2.17	0.45
1:A:29:PHE:O	1:A:96:THR:HA	2.17	0.45
1:L:49:VAL:O	1:L:110:SER:HA	2.16	0.44
1:K:49:VAL:O	1:K:110:SER:HA	2.17	0.44
1:H:4:SER:HA	1:H:30:THR:O	2.17	0.44
1:F:87:ILE:HB	1:F:91:GLU:HB2	1.99	0.44
1:K:8:GLN:HG2	1:K:34:SER:OG	2.16	0.44
1:B:74:LYS:O	1:B:77:ASP:HB2	2.17	0.44
1:K:92:LYS:HE2	3:K:630:HOH:O	2.17	0.44
1:F:104:GLU:HB2	3:F:2748:HOH:O	2.17	0.44
1:I:46:HIS:CE1	1:I:121:MET:HE3	2.53	0.44
1:D:118:SER:O	1:D:122:LYS:HE3	2.18	0.43
1:G:75:PRO:HA	3:G:1831:HOH:O	2.18	0.43
1:H:21:THR:HA	1:H:126:THR:O	2.18	0.43
1:H:7:ILE:HD11	1:H:15:PHE:HB3	2.00	0.43
1:I:87:ILE:HB	1:I:91:GLU:HB2	2.00	0.43
1:M:1:ALA:HB3	1:M:4:SER:OG	2.18	0.43
1:K:29:PHE:O	1:K:96:THR:HA	2.18	0.43
1:H:64:MET:HG3	1:H:115:PRO:HG3	2.00	0.43
1:B:33:LEU:HG	1:B:87:ILE:HD11	2.00	0.43
1:G:48:TRP:O	1:G:83:HIS:HA	2.19	0.42
1:D:87:ILE:HB	1:D:91:GLU:HB2	2.01	0.42
1:D:85:LYS:HB2	1:D:85:LYS:NZ	2.34	0.42
1:D:11:ASP:HA	1:D:44:MET:HG2	2.02	0.42
1:A:64:MET:HB2	3:A:578:HOH:O	2.18	0.42
1:L:102:LEU:HD12	3:L:2808:HOH:O	2.19	0.42
1:L:13:MET:CE	1:L:117:HIS:HA	2.49	0.42
1:G:49:VAL:O	1:G:110:SER:HA	2.20	0.42
1:C:48:TRP:O	1:C:83:HIS:HA	2.20	0.41
1:M:13:MET:HE3	1:M:117:HIS:HA	2.02	0.41
1:C:107:GLN:HA	3:C:2058:HOH:O	2.20	0.41
1:B:49:VAL:O	1:B:110:SER:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:33:LEU:HG	1:K:87:ILE:HD11	2.02	0.41
1:E:58:GLY:HA2	3:E:2905:HOH:O	2.20	0.41
1:D:15:PHE:CD1	1:D:121:MET:HE2	2.56	0.41
1:F:114:PHE:O	1:F:117:HIS:HB2	2.21	0.41
1:E:22:VAL:O	1:E:127:LEU:HD23	2.20	0.41
1:K:31:VAL:O	1:K:94:SER:HA	2.21	0.41
1:D:53:ALA:HA	1:D:109:MET:HG3	2.04	0.40
1:E:4:SER:HA	1:E:30:THR:O	2.21	0.40
1:A:48:TRP:O	1:A:83:HIS:HA	2.21	0.40
1:L:74:LYS:NZ	1:L:77:ASP:HA	2.37	0.40
1:C:50:LEU:HD13	1:C:125:LEU:HD13	2.04	0.40

All (3) 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:D:70:LYS:HZ2	3:D:1944:HOH:H2[1_455]	1.32	0.28
1:C:79:ARG:HH12	3:K:2351:HOH:H1[2_646]	1.34	0.26
1:G:12:GLN:HE21	1:I:85:LYS:HZ3[1_554]	1.34	0.26

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	126/128 (98%)	117 (93%)	9 (7%)	0	100	100
1	B	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
1	C	126/128 (98%)	121 (96%)	5 (4%)	0	100	100
1	D	126/128 (98%)	122 (97%)	3 (2%)	1 (1%)	24	27
1	E	126/128 (98%)	119 (94%)	7 (6%)	0	100	100
1	F	126/128 (98%)	121 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	G	126/128 (98%)	118 (94%)	7 (6%)	1 (1%)	24 27
1	H	126/128 (98%)	120 (95%)	6 (5%)	0	100 100
1	I	126/128 (98%)	122 (97%)	4 (3%)	0	100 100
1	K	126/128 (98%)	123 (98%)	3 (2%)	0	100 100
1	L	126/128 (98%)	122 (97%)	4 (3%)	0	100 100
1	M	126/128 (98%)	122 (97%)	4 (3%)	0	100 100
All	All	1512/1536 (98%)	1450 (96%)	60 (4%)	2 (0%)	56 68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	3	CYS
1	D	13	MET

5.3.2 Protein sidechains (i)

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	110/110 (100%)	104 (94%)	6 (6%)	27 36
1	B	110/110 (100%)	109 (99%)	1 (1%)	84 93
1	C	110/110 (100%)	102 (93%)	8 (7%)	17 22
1	D	110/110 (100%)	102 (93%)	8 (7%)	17 22
1	E	110/110 (100%)	104 (94%)	6 (6%)	27 36
1	F	110/110 (100%)	102 (93%)	8 (7%)	17 22
1	G	110/110 (100%)	104 (94%)	6 (6%)	27 36
1	H	110/110 (100%)	103 (94%)	7 (6%)	22 28
1	I	110/110 (100%)	103 (94%)	7 (6%)	22 28
1	K	110/110 (100%)	108 (98%)	2 (2%)	66 82
1	L	110/110 (100%)	103 (94%)	7 (6%)	22 28
1	M	110/110 (100%)	108 (98%)	2 (2%)	66 82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1320/1320 (100%)	1252 (95%)	68 (5%)	29 38

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	PHE
1	A	75	PRO
1	A	110	SER
1	A	118	SER
1	A	126	THR
1	A	127	LEU
1	B	94	SER
1	C	25	SER
1	C	35	HIS
1	C	98	ASP
1	C	100	SER
1	C	107	GLN
1	C	122	LYS
1	C	127	LEU
1	C	128	LYS
1	D	8	GLN
1	D	12	GLN
1	D	25	SER
1	D	27	LYS
1	D	85	LYS
1	D	103	LYS
1	D	106	GLU
1	D	128	LYS
1	E	15	PHE
1	E	38	ASN
1	E	106	GLU
1	E	107	GLN
1	E	125	LEU
1	E	127	LEU
1	F	15	PHE
1	F	35	HIS
1	F	69	ASP
1	F	85	LYS
1	F	107	GLN
1	F	118	SER
1	F	122	LYS
1	F	125	LEU

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Mol	Chain	Res	Type
1	G	6	ASP
1	G	28	GLN
1	G	69	ASP
1	G	76	ASP
1	G	107	GLN
1	G	122	LYS
1	H	25	SER
1	H	34	SER
1	H	38	ASN
1	H	78	SER
1	H	120	LEU
1	H	122	LYS
1	H	128	LYS
1	I	38	ASN
1	I	100	SER
1	I	103	LYS
1	I	106	GLU
1	I	118	SER
1	I	125	LEU
1	I	128	LYS
1	K	38	ASN
1	K	122	LYS
1	L	15	PHE
1	L	28	GLN
1	L	35	HIS
1	L	38	ASN
1	L	44	MET
1	L	118	SER
1	L	122	LYS
1	M	85	LYS
1	M	126	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	B	8	GLN
1	C	107	GLN
1	D	28	GLN
1	F	28	GLN
1	F	32	ASN
1	G	107	GLN

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Mol	Chain	Res	Type
1	H	8	GLN
1	L	8	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 12 ligands modelled in this entry, 12 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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.