Full wwPDB X-ray Structure Validation Report (i)

Jan 27, 2024 – 10:11 AM EST

PDB ID	:	1AZN
Title	:	CRYSTAL STRUCTURE OF THE AZURIN MUTANT PHE114ALA FROM PSEUDOMONAS AERUGINOSA AT 2.6 ANGSTROMS RESOLUTION
Authors	:	Tsai, L.-C.; Sjolin, L.; Langer, V.; Pascher, T.; Nar, H.
Deposited on	:	1994-05-27
Resolution	:	2.60 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

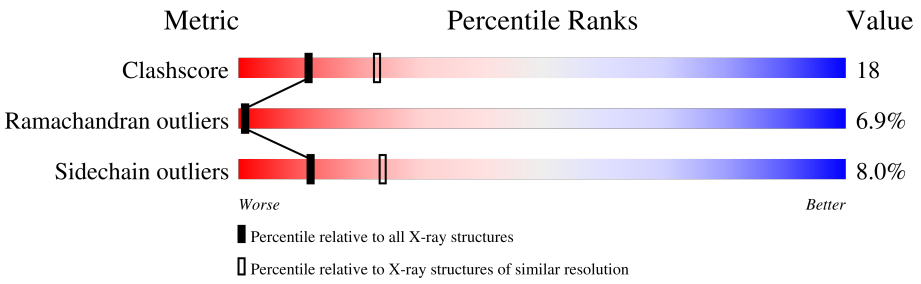
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 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	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	128	42% 41% 15% •
1	B	128	45% 42% 8% 5%
1	C	128	49% 32% 16% •
1	D	128	42% 38% 16% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4312 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 AZURIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	128	967	601	164	193	9	0	0	0
1	B	128	967	601	164	193	9	0	0	0
1	C	128	967	601	164	193	9	0	0	0
1	D	128	967	601	164	193	9	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	114	ALA	PHE	conflict	UNP P00282
B	114	ALA	PHE	conflict	UNP P00282
C	114	ALA	PHE	conflict	UNP P00282
D	114	ALA	PHE	conflict	UNP P00282

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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	103	103	103	0	0
			Total	O		
3	B	113	113	113	0	0
			Total	O		
3	C	122	122	122	0	0
			Total	O		
3	D	102	102	102	0	0

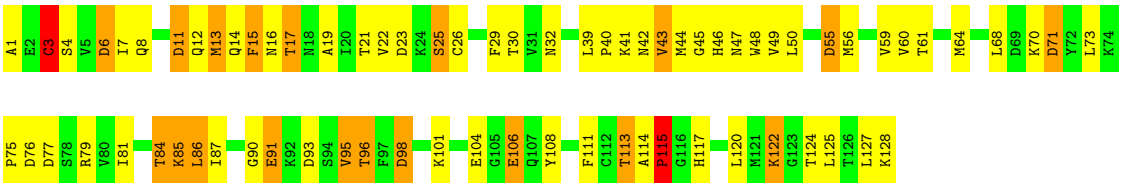
3 Residue-property plots (i)

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

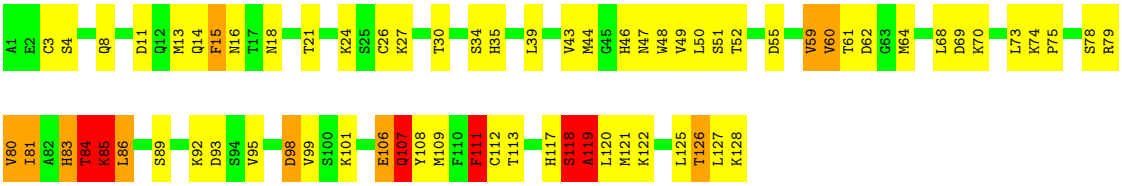
• Molecule 1: AZURIN

Chain A: 42% 41% 15% •



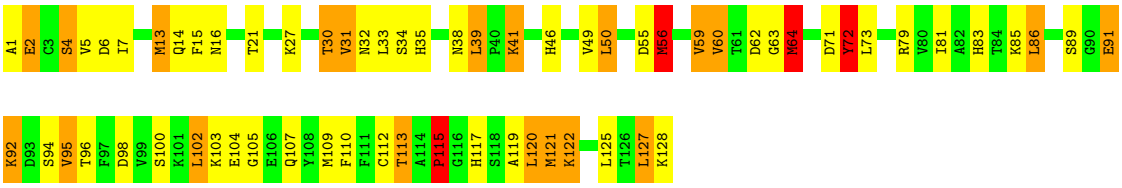
• Molecule 1: AZURIN

Chain B: 45% 42% 8% 5%



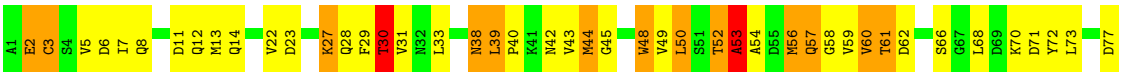
• Molecule 1: AZURIN

Chain C: 49% 32% 16% •



• Molecule 1: AZURIN

Chain D: 42% 38% 16% •



S78
R79
V80
I81
A82
H83
T84
K85
L86
I87
K92
D93
S94
V95
T96
F97
L102
K103
E104
G105
E106
Q107
Y108
M109
F110
F111
C112
P115
G116
H117
S118
A119
L120
M121
K122
L125
T126
L127
K128

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	51.00Å 83.60Å 66.40Å 90.00° 110.50° 90.00°	Depositor
Resolution (Å)	8.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.185 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4312	wwPDB-VP
Average B, all atoms ($Å^2$)	26.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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	2.64	4/983 (0.4%)	2.45	40/1326 (3.0%)
1	B	1.14	2/983 (0.2%)	2.05	36/1326 (2.7%)
1	C	1.16	3/983 (0.3%)	2.08	39/1326 (2.9%)
1	D	1.19	6/983 (0.6%)	2.17	45/1326 (3.4%)
All	All	1.66	15/3932 (0.4%)	2.19	160/5304 (3.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	CYS	C-O	73.91	2.63	1.23
1	A	3	CYS	CA-C	-8.72	1.30	1.52
1	B	108	TYR	CE2-CZ	8.52	1.49	1.38
1	C	62	ASP	C-N	8.37	1.48	1.33
1	D	60	VAL	N-CA	8.21	1.62	1.46
1	A	19	ALA	N-CA	8.11	1.62	1.46
1	D	52	THR	N-CA	8.05	1.62	1.46
1	B	108	TYR	CE1-CZ	-7.39	1.28	1.38
1	C	2	GLU	N-CA	6.52	1.59	1.46
1	D	6	ASP	N-CA	6.47	1.59	1.46
1	D	5	VAL	N-CA	5.74	1.57	1.46
1	C	14	GLN	CD-OE1	5.36	1.35	1.24
1	A	6	ASP	N-CA	5.29	1.56	1.46
1	D	128	LYS	CA-CB	-5.29	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	44	MET	SD-CE	5.22	2.07	1.77

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3	CYS	CB-CA-C	29.81	170.02	110.40
1	A	3	CYS	CA-C-O	-25.21	67.17	120.10
1	A	3	CYS	CA-C-N	23.27	168.39	117.20
1	A	3	CYS	N-CA-C	-12.96	76.00	111.00
1	D	128	LYS	CA-CB-CG	11.78	139.31	113.40
1	A	76	ASP	CB-CG-OD1	9.51	126.86	118.30
1	A	15	PHE	CA-CB-CG	9.47	136.63	113.90
1	C	39	LEU	CA-CB-CG	9.41	136.96	115.30
1	B	113	THR	CA-CB-CG2	9.32	125.45	112.40
1	D	58	GLY	O-C-N	9.24	137.49	122.70
1	B	14	GLN	CA-CB-CG	9.13	133.48	113.40
1	D	79	ARG	CD-NE-CZ	8.99	136.18	123.60
1	C	85	LYS	CA-CB-CG	8.78	132.71	113.40
1	B	112	CYS	CA-CB-SG	8.74	129.73	114.00
1	A	44	MET	CA-CB-CG	8.69	128.07	113.30
1	D	27	LYS	CA-CB-CG	8.67	132.46	113.40
1	D	30	THR	CA-CB-CG2	8.66	124.53	112.40
1	B	83	HIS	CA-CB-CG	8.60	128.22	113.60
1	B	13	MET	CA-CB-CG	8.34	127.48	113.30
1	A	14	GLN	CA-CB-CG	8.23	131.51	113.40
1	C	102	LEU	CA-CB-CG	8.18	134.11	115.30
1	C	55	ASP	CB-CG-OD1	8.13	125.62	118.30
1	A	85	LYS	CA-CB-CG	8.10	131.21	113.40
1	B	106	GLU	N-CA-CB	8.04	125.06	110.60
1	C	112	CYS	CA-CB-SG	8.01	128.41	114.00
1	D	44	MET	N-CA-CB	-7.98	96.23	110.60
1	A	128	LYS	CA-CB-CG	7.95	130.89	113.40
1	D	79	ARG	NE-CZ-NH2	7.91	124.26	120.30
1	D	109	MET	CA-CB-CG	7.88	126.70	113.30
1	B	68	LEU	CA-CB-CG	7.78	133.19	115.30
1	B	117	HIS	CA-CB-CG	7.77	126.80	113.60
1	A	79	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	D	53	ALA	N-CA-CB	-7.66	99.38	110.10
1	C	64	MET	N-CA-CB	-7.65	96.83	110.60
1	D	72	TYR	N-CA-CB	7.61	124.30	110.60
1	D	85	LYS	CA-CB-CG	7.58	130.07	113.40
1	D	72	TYR	CB-CG-CD2	-7.49	116.50	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	91	GLU	CA-CB-CG	7.40	129.69	113.40
1	B	55	ASP	CB-CG-OD1	7.37	124.94	118.30
1	A	17	THR	CA-C-O	7.32	135.47	120.10
1	C	39	LEU	CB-CG-CD2	7.28	123.38	111.00
1	D	72	TYR	CB-CG-CD1	7.27	125.36	121.00
1	C	110	PHE	CA-CB-CG	7.25	131.30	113.90
1	D	93	ASP	CB-CG-OD1	7.24	124.82	118.30
1	A	17	THR	CA-C-N	-7.22	101.32	117.20
1	A	55	ASP	CB-CG-OD1	7.18	124.76	118.30
1	A	70	LYS	CA-CB-CG	7.17	129.16	113.40
1	A	122	LYS	CA-CB-CG	7.13	129.09	113.40
1	C	27	LYS	CA-CB-CG	7.07	128.96	113.40
1	A	86	LEU	CA-CB-CG	7.03	131.47	115.30
1	C	107	GLN	CA-CB-CG	6.97	128.74	113.40
1	D	58	GLY	CA-C-N	-6.95	101.92	117.20
1	D	3	CYS	C-N-CA	6.92	139.00	121.70
1	A	12	GLN	CB-CG-CD	6.91	129.56	111.60
1	D	77	ASP	N-CA-CB	6.88	122.98	110.60
1	B	128	LYS	CA-CB-CG	6.84	128.44	113.40
1	C	62	ASP	CA-CB-CG	6.82	128.40	113.40
1	B	27	LYS	N-CA-CB	6.79	122.82	110.60
1	C	2	GLU	N-CA-C	6.79	129.32	111.00
1	B	18	ASN	CA-CB-CG	6.71	128.16	113.40
1	B	83	HIS	N-CA-CB	6.66	122.59	110.60
1	D	94	SER	N-CA-CB	6.63	120.45	110.50
1	A	98	ASP	CB-CG-OD1	6.63	124.27	118.30
1	A	6	ASP	N-CA-C	-6.57	93.26	111.00
1	D	11	ASP	C-N-CA	6.48	137.90	121.70
1	D	62	ASP	CB-CG-OD2	6.48	124.13	118.30
1	A	120	LEU	CA-CB-CG	6.44	130.12	115.30
1	B	107	GLN	C-N-CA	-6.38	105.74	121.70
1	C	2	GLU	N-CA-CB	-6.34	99.18	110.60
1	C	113	THR	CA-CB-CG2	6.33	121.27	112.40
1	B	109	MET	CA-CB-CG	6.31	124.03	113.30
1	B	80	VAL	CB-CA-C	6.28	123.33	111.40
1	C	56	MET	CG-SD-CE	6.22	110.15	100.20
1	B	34	SER	N-CA-CB	6.17	119.75	110.50
1	D	39	LEU	CA-CB-CG	6.16	129.47	115.30
1	A	98	ASP	CA-CB-CG	6.16	126.95	113.40
1	A	86	LEU	CB-CA-C	6.11	121.82	110.20
1	B	79	ARG	CD-NE-CZ	6.11	132.16	123.60
1	D	50	LEU	O-C-N	6.11	132.47	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	86	LEU	CA-CB-CG	6.10	129.33	115.30
1	D	112	CYS	CA-CB-SG	6.10	124.98	114.00
1	D	122	LYS	CA-CB-CG	6.06	126.74	113.40
1	C	120	LEU	CA-CB-CG	6.03	129.17	115.30
1	C	95	VAL	N-CA-CB	6.03	124.76	111.50
1	A	41	LYS	CG-CD-CE	6.02	129.95	111.90
1	D	44	MET	CG-SD-CE	-6.01	90.59	100.20
1	D	6	ASP	CA-CB-CG	5.96	126.51	113.40
1	A	47	ASN	N-CA-CB	5.87	121.16	110.60
1	D	48	TRP	CA-CB-CG	5.86	124.84	113.70
1	A	59	VAL	CA-CB-CG1	5.86	119.69	110.90
1	B	119	ALA	N-CA-C	5.85	126.79	111.00
1	C	86	LEU	CB-CA-C	5.81	121.25	110.20
1	C	109	MET	CA-CB-CG	5.79	123.14	113.30
1	B	84	THR	CA-CB-CG2	5.75	120.44	112.40
1	A	95	VAL	O-C-N	5.73	131.87	122.70
1	B	84	THR	N-CA-CB	5.71	121.14	110.30
1	C	15	PHE	N-CA-CB	5.69	120.83	110.60
1	D	93	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	C	92	LYS	CA-CB-CG	5.67	125.86	113.40
1	B	119	ALA	N-CA-CB	-5.66	102.18	110.10
1	B	60	VAL	CB-CA-C	5.63	122.10	111.40
1	D	44	MET	N-CA-C	5.62	126.19	111.00
1	C	1	ALA	CB-CA-C	5.60	118.49	110.10
1	B	81	ILE	CB-CA-C	5.59	122.77	111.60
1	C	50	LEU	N-CA-CB	5.58	121.56	110.40
1	B	70	LYS	CA-CB-CG	5.58	125.67	113.40
1	B	127	LEU	CB-CA-C	5.55	120.75	110.20
1	C	15	PHE	CA-CB-CG	5.55	127.23	113.90
1	C	98	ASP	CB-CG-OD2	5.55	123.30	118.30
1	A	128	LYS	N-CA-CB	5.54	120.58	110.60
1	B	15	PHE	CA-CB-CG	5.53	127.17	113.90
1	A	77	ASP	N-CA-CB	5.53	120.55	110.60
1	C	122	LYS	CA-CB-CG	5.52	125.54	113.40
1	D	83	HIS	N-CA-CB	5.51	120.53	110.60
1	A	15	PHE	N-CA-CB	5.51	120.52	110.60
1	B	118	SER	N-CA-CB	5.51	118.76	110.50
1	B	85	LYS	CA-CB-CG	5.47	125.44	113.40
1	C	91	GLU	OE1-CD-OE2	-5.47	116.73	123.30
1	D	38	ASN	CA-CB-CG	5.45	125.39	113.40
1	A	6	ASP	CB-CA-C	5.44	121.29	110.40
1	A	76	ASP	CA-CB-CG	5.44	125.36	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	127	LEU	CA-CB-CG	5.44	127.81	115.30
1	C	38	ASN	N-CA-C	5.42	125.64	111.00
1	C	85	LYS	N-CA-CB	5.41	120.34	110.60
1	D	52	THR	C-N-CA	-5.39	108.22	121.70
1	A	59	VAL	CB-CA-C	5.32	121.51	111.40
1	D	42	ASN	CA-CB-CG	5.32	125.10	113.40
1	C	91	GLU	CA-CB-CG	5.31	125.09	113.40
1	D	86	LEU	CB-CA-C	5.30	120.28	110.20
1	B	122	LYS	CA-CB-CG	5.30	125.06	113.40
1	C	6	ASP	N-CA-CB	5.29	120.12	110.60
1	D	53	ALA	N-CA-C	5.29	125.27	111.00
1	C	4	SER	N-CA-CB	5.28	118.43	110.50
1	D	12	GLN	C-N-CA	5.28	134.91	121.70
1	B	47	ASN	CB-CA-C	5.27	120.94	110.40
1	C	72	TYR	CA-CB-CG	5.24	123.36	113.40
1	A	45	GLY	CA-C-O	5.23	130.01	120.60
1	A	11	ASP	CB-CG-OD2	5.23	123.00	118.30
1	D	77	ASP	CA-C-N	-5.22	105.72	117.20
1	B	111	PHE	CB-CG-CD1	5.20	124.44	120.80
1	B	62	ASP	CB-CA-C	5.19	120.78	110.40
1	C	41	LYS	CG-CD-CE	5.19	127.47	111.90
1	C	112	CYS	N-CA-CB	5.17	119.91	110.60
1	A	106	GLU	OE1-CD-OE2	5.17	129.50	123.30
1	C	127	LEU	CA-CB-CG	5.15	127.15	115.30
1	D	57	GLN	CB-CA-C	5.15	120.70	110.40
1	C	79	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	C	79	ARG	CD-NE-CZ	5.13	130.78	123.60
1	D	108	TYR	CB-CG-CD2	5.12	124.07	121.00
1	A	101	LYS	C-N-CA	5.10	134.45	121.70
1	D	80	VAL	CB-CA-C	5.08	121.05	111.40
1	D	85	LYS	N-CA-CB	5.07	119.73	110.60
1	D	93	ASP	CB-CA-C	5.05	120.50	110.40
1	B	98	ASP	N-CA-CB	5.04	119.67	110.60
1	A	6	ASP	CA-C-O	-5.04	109.53	120.10
1	C	31	VAL	CA-CB-CG2	5.03	118.45	110.90
1	D	56	MET	CA-CB-CG	5.02	121.84	113.30
1	D	2	GLU	CG-CD-OE1	5.01	128.33	118.30
1	B	79	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	A	77	ASP	CB-CG-OD1	5.01	122.81	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	3	CYS	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3	CYS	Mainchain,Peptide

5.2 Too-close contacts (i)

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	967	0	950	42	0
1	B	967	0	950	27	0
1	C	967	0	950	27	0
1	D	967	0	948	39	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
3	A	103	0	0	0	0
3	B	113	0	0	0	0
3	C	122	0	0	0	0
3	D	102	0	0	1	0
All	All	4312	0	3798	135	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 18.

All (135) 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:D:44:MET:CE	1:D:44:MET:SD	2.07	1.41
1:A:7:ILE:HG13	1:A:16:ASN:OD1	1.57	1.04
1:D:52:THR:HA	1:D:107:GLN:O	1.72	0.90
1:A:60:VAL:HA	1:A:113:THR:HG22	1.56	0.87
1:A:39:LEU:HD22	1:A:43:VAL:HG11	1.66	0.76
1:D:30:THR:OG1	1:D:96:THR:HG23	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ILE:HA	1:A:16:ASN:HD21	1.50	0.75
1:D:49:VAL:HG13	1:D:80:VAL:HG13	1.68	0.74
1:A:1:ALA:HB3	1:A:4:SER:OG	1.89	0.72
1:A:50:LEU:HD11	1:A:125:LEU:HD22	1.72	0.72
1:A:13:MET:SD	1:A:117:HIS:CD2	2.84	0.70
1:B:49:VAL:HG21	1:B:73:LEU:HD21	1.72	0.69
1:D:23:ASP:HA	1:D:128:LYS:HG2	1.74	0.69
1:B:84:THR:HG22	1:B:95:VAL:HG12	1.75	0.68
1:A:6:ASP:HA	1:A:32:ASN:HB2	1.77	0.67
1:A:3:CYS:CA	1:A:3:CYS:O	2.44	0.65
1:B:35:HIS:CE1	1:B:89:SER:HB3	2.31	0.65
1:B:49:VAL:HG11	1:B:59:VAL:HG11	1.78	0.65
1:C:50:LEU:HD11	1:C:125:LEU:HD22	1.79	0.65
1:D:13:MET:HE2	1:D:120:LEU:HD12	1.80	0.63
1:D:44:MET:CE	1:D:44:MET:CG	2.76	0.63
1:C:30:THR:HG1	1:C:96:THR:HG1	1.38	0.62
1:A:60:VAL:HA	1:A:113:THR:CG2	2.28	0.62
1:A:8:GLN:HB2	1:A:16:ASN:HB3	1.81	0.62
1:C:50:LEU:HD23	1:C:81:ILE:HB	1.82	0.60
1:D:103:LYS:HA	3:D:848:HOH:O	2.01	0.60
1:A:1:ALA:C	1:A:4:SER:OG	2.40	0.59
1:D:2:GLU:HG2	1:D:3:CYS:SG	2.42	0.59
1:A:68:LEU:HD12	1:A:86:LEU:HD21	1.85	0.58
1:D:39:LEU:HB3	1:D:40:PRO:HD2	1.86	0.58
1:A:7:ILE:CG1	1:A:16:ASN:OD1	2.42	0.57
1:A:46:HIS:O	1:A:86:LEU:HA	2.04	0.57
1:A:42:ASN:HD21	1:A:43:VAL:HG23	1.69	0.56
1:D:66:SER:HB3	1:D:70:LYS:HB2	1.88	0.56
1:B:39:LEU:HD22	1:B:43:VAL:HG11	1.87	0.56
1:B:106:GLU:HG2	1:B:107:GLN:H	1.71	0.56
1:B:4:SER:HB3	1:B:30:THR:HG23	1.89	0.55
1:D:102:LEU:HD13	1:D:125:LEU:HD21	1.88	0.54
1:A:1:ALA:CB	1:A:4:SER:OG	2.55	0.54
1:B:74:LYS:HG2	1:B:75:PRO:HD2	1.90	0.53
1:D:52:THR:O	1:D:54:ALA:N	2.41	0.53
1:D:53:ALA:HB2	1:D:109:MET:HG2	1.90	0.53
1:B:46:HIS:CE1	1:B:121:MET:SD	3.02	0.53
1:B:98:ASP:H	1:B:101:LYS:HE3	1.74	0.53
1:C:49:VAL:HG21	1:C:113:THR:HG23	1.89	0.52
1:A:7:ILE:CD1	1:A:17:THR:HG22	2.39	0.52
1:D:31:VAL:HG21	1:D:48:TRP:CZ2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:LEU:HB3	1:C:127:LEU:HG	1.91	0.52
1:A:3:CYS:HG	1:A:26:CYS:HG	1.57	0.52
1:A:114:ALA:O	1:A:117:HIS:HB2	2.10	0.52
1:D:44:MET:SD	1:D:117:HIS:CE1	3.03	0.52
1:C:30:THR:OG1	1:C:96:THR:OG1	2.16	0.51
1:C:102:LEU:HD12	1:C:127:LEU:HD23	1.93	0.51
1:C:32:ASN:HB3	1:C:92:LYS:HE3	1.93	0.51
1:D:45:GLY:HA2	1:D:87:ILE:O	2.11	0.51
1:A:104:GLU:HB2	1:A:127:LEU:HD12	1.94	0.50
1:C:71:ASP:OD1	1:C:86:LEU:HB3	2.11	0.50
1:D:85:LYS:O	1:D:87:ILE:HG23	2.12	0.50
1:D:57:GLN:O	1:D:61:THR:HB	2.11	0.49
1:C:34:SER:HB3	1:C:92:LYS:HD3	1.93	0.49
1:A:11:ASP:OD1	1:A:39:LEU:HB2	2.13	0.49
1:A:8:GLN:N	1:A:16:ASN:ND2	2.61	0.49
1:A:22:VAL:HG13	1:A:29:PHE:CD1	2.49	0.48
1:C:4:SER:HB3	1:C:30:THR:HG22	1.95	0.48
1:D:13:MET:HG3	1:D:44:MET:SD	2.54	0.48
1:D:102:LEU:O	1:D:127:LEU:HG	2.14	0.48
1:A:64:MET:HG3	1:A:115:PRO:HG3	1.95	0.48
1:B:92:LYS:O	1:B:93:ASP:HB2	2.14	0.48
1:A:7:ILE:HD12	1:A:17:THR:HG22	1.96	0.47
1:A:42:ASN:ND2	1:A:43:VAL:HG23	2.30	0.47
1:B:52:THR:HA	1:B:107:GLN:O	2.15	0.47
1:B:8:GLN:HB2	1:B:16:ASN:HB3	1.97	0.47
1:B:61:THR:O	1:B:64:MET:HB3	2.15	0.47
1:A:8:GLN:H	1:A:16:ASN:ND2	2.13	0.47
1:A:29:PHE:O	1:A:96:THR:HA	2.15	0.47
1:C:13:MET:C	1:C:121:MET:HE3	2.35	0.47
1:D:40:PRO:HG2	1:D:43:VAL:HB	1.97	0.46
1:B:15:PHE:HE2	1:B:111:PHE:HA	1.81	0.46
1:C:117:HIS:HB3	1:C:121:MET:HG3	1.97	0.46
1:D:71:ASP:OD1	1:D:86:LEU:HB3	2.15	0.46
1:A:3:CYS:O	1:A:3:CYS:HA	2.16	0.46
1:A:87:ILE:HB	1:A:91:GLU:HB2	1.98	0.46
1:B:50:LEU:HD23	1:B:81:ILE:HG22	1.97	0.46
1:D:27:LYS:O	1:D:28:GLN:HG3	2.16	0.45
1:D:39:LEU:HD13	1:D:43:VAL:HG11	1.99	0.45
1:C:5:VAL:HG13	1:C:31:VAL:HG13	1.98	0.45
1:C:56:MET:O	1:C:59:VAL:HB	2.17	0.45
1:A:23:ASP:OD2	1:A:25:SER:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ASP:HB3	1:A:86:LEU:HB3	1.98	0.45
1:D:56:MET:O	1:D:60:VAL:N	2.44	0.45
1:C:7:ILE:HA	1:C:16:ASN:OD1	2.17	0.45
1:B:11:ASP:HA	1:B:44:MET:HG2	1.99	0.45
1:B:92:LYS:HG3	1:B:93:ASP:H	1.82	0.45
1:A:50:LEU:HD23	1:A:81:ILE:HG22	1.99	0.44
1:D:50:LEU:HD11	1:D:125:LEU:HD13	1.99	0.44
1:B:26:CYS:HB3	1:B:99:VAL:HG21	2.00	0.44
1:C:35:HIS:HB3	1:C:89:SER:HA	1.99	0.44
1:A:1:ALA:C	1:A:4:SER:HG	2.22	0.44
1:D:80:VAL:HG11	1:D:83:HIS:CD2	2.53	0.44
1:C:21:THR:HG22	1:C:128:LYS:HG2	1.99	0.43
1:C:104:GLU:HA	1:C:127:LEU:HD12	2.01	0.43
1:D:50:LEU:CD1	1:D:125:LEU:HD13	2.49	0.43
1:D:22:VAL:HG22	1:D:29:PHE:CZ	2.53	0.43
1:D:68:LEU:HD12	1:D:86:LEU:HD21	2.00	0.43
1:A:106:GLU:HG2	1:A:108:TYR:CZ	2.54	0.43
1:B:46:HIS:O	1:B:86:LEU:HD12	2.19	0.43
1:D:48:TRP:HZ3	1:D:82:ALA:HB3	1.83	0.43
1:A:49:VAL:HG21	1:A:73:LEU:HD21	2.00	0.43
1:C:72:TYR:CE2	1:C:115:PRO:HD2	2.54	0.43
1:C:32:ASN:HA	1:C:94:SER:OG	2.19	0.42
1:B:85:LYS:HG2	1:B:93:ASP:OD2	2.20	0.42
1:A:30:THR:HA	1:A:95:VAL:O	2.19	0.42
1:A:15:PHE:HE2	1:A:111:PHE:HA	1.85	0.42
1:D:80:VAL:CG1	1:D:83:HIS:HD2	2.33	0.42
1:C:46:HIS:CE1	1:C:121:MET:SD	3.13	0.42
1:C:60:VAL:O	1:C:64:MET:N	2.45	0.41
1:B:21:THR:HA	1:B:126:THR:HG23	2.02	0.41
1:D:29:PHE:O	1:D:96:THR:HA	2.21	0.41
1:D:33:LEU:O	1:D:92:LYS:HG3	2.20	0.41
1:D:13:MET:CE	1:D:117:HIS:HA	2.50	0.41
1:B:48:TRP:HB3	1:B:84:THR:HG23	2.03	0.41
1:C:83:HIS:H	1:C:95:VAL:HG11	1.86	0.41
1:D:49:VAL:HG11	1:D:59:VAL:HG11	2.03	0.41
1:A:55:ASP:O	1:A:56:MET:C	2.59	0.41
1:C:33:LEU:O	1:C:92:LYS:HD2	2.21	0.41
1:A:48:TRP:HB3	1:A:84:THR:HG23	2.03	0.40
1:B:11:ASP:OD1	1:B:39:LEU:HB2	2.20	0.40
1:B:49:VAL:HG13	1:B:80:VAL:HG13	2.04	0.40
1:C:119:ALA:C	1:C:120:LEU:HD23	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:LEU:HD22	1:D:80:VAL:HG21	2.02	0.40
1:D:97:PHE:HE2	1:D:102:LEU:HD11	1.86	0.40
1:A:85:LYS:HG2	1:A:93:ASP:OD2	2.21	0.40
1:B:118:SER:O	1:B:119:ALA:C	2.60	0.40
1:B:24:LYS:C	1:B:26:CYS:H	2.24	0.40
1:C:59:VAL:O	1:C:63:GLY:N	2.49	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	126/128 (98%)	99 (79%)	17 (14%)	10 (8%)	1	1
1	B	126/128 (98%)	99 (79%)	19 (15%)	8 (6%)	1	1
1	C	126/128 (98%)	95 (75%)	20 (16%)	11 (9%)	1	0
1	D	126/128 (98%)	101 (80%)	19 (15%)	6 (5%)	2	2
All	All	504/512 (98%)	394 (78%)	75 (15%)	35 (7%)	1	1

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	ASP
1	B	83	HIS
1	B	118	SER
1	B	119	ALA
1	C	2	GLU
1	C	59	VAL
1	D	83	HIS
1	A	3	CYS
1	A	13	MET

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Mol	Chain	Res	Type
1	C	56	MET
1	C	60	VAL
1	C	64	MET
1	C	100	SER
1	C	105	GLY
1	D	103	LYS
1	D	105	GLY
1	A	25	SER
1	A	90	GLY
1	A	115	PRO
1	B	51	SER
1	C	13	MET
1	C	91	GLU
1	D	53	ALA
1	A	40	PRO
1	A	61	THR
1	B	3	CYS
1	A	43	VAL
1	C	72	TYR
1	C	115	PRO
1	D	111	PHE
1	B	59	VAL
1	B	111	PHE
1	B	60	VAL
1	A	75	PRO
1	D	115	PRO

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	109/109 (100%)	101 (93%)	8 (7%)	14 28
1	B	109/109 (100%)	101 (93%)	8 (7%)	14 28
1	C	109/109 (100%)	101 (93%)	8 (7%)	14 28
1	D	109/109 (100%)	98 (90%)	11 (10%)	7 14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	436/436 (100%)	401 (92%)	35 (8%)	12 24

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	THR
1	A	84	THR
1	A	96	THR
1	A	98	ASP
1	A	113	THR
1	A	115	PRO
1	A	122	LYS
1	A	124	THR
1	B	69	ASP
1	B	78	SER
1	B	84	THR
1	B	85	LYS
1	B	107	GLN
1	B	120	LEU
1	B	125	LEU
1	B	126	THR
1	C	30	THR
1	C	39	LEU
1	C	41	LYS
1	C	73	LEU
1	C	103	LYS
1	C	115	PRO
1	C	121	MET
1	C	122	LYS
1	D	7	ILE
1	D	8	GLN
1	D	14	GLN
1	D	30	THR
1	D	38	ASN
1	D	61	THR
1	D	78	SER
1	D	96	THR
1	D	118	SER
1	D	122	LYS
1	D	127	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	42	ASN
1	A	57	GLN
1	A	117	HIS
1	B	107	GLN
1	D	8	GLN
1	D	28	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.