Full wwPDB X-ray Structure Validation Report (i)

Apr 30, 2025 – 02:10 AM EDT

PDB ID	:	3DSG / pdb_00003dsg
Title	:	XC1028 from Xanthomonas campestris Adopts a PilZ Domain-like Structure Yet with Trivial c-di-GMP Binding Activity
Authors	:	Li, T.N.; Chin, K.H.; Liu, J.H.; Wang, A.H.J.; Chou, S.H.
Deposited on	:	2008-07-12
Resolution	:	2.09 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:

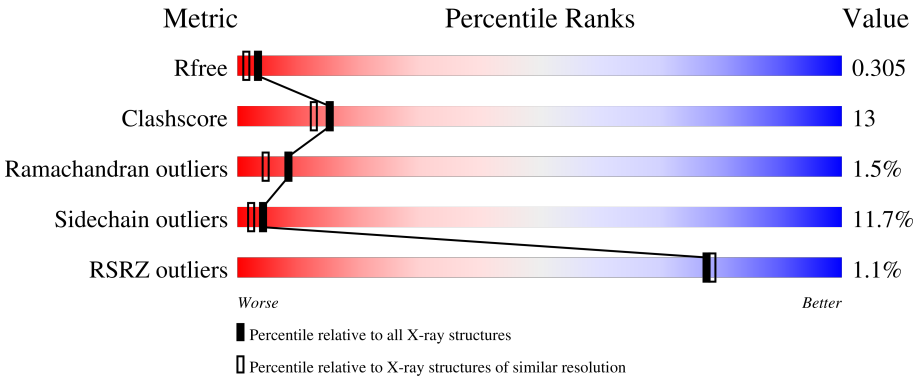
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.09 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}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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 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% 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	99	18% 53% 21% • 5%
1	B	99	2% 27% 45% 19% 6% •
1	C	99	% 21% 46% 22% 5% 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2263 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 Type IV fimbriae assembly protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	94	Total	C	N	O	Se	0	0	0
			710	461	117	130	2			
1	B	97	Total	C	N	O	Se	0	0	0
			724	469	120	133	2			
1	C	94	Total	C	N	O	Se	0	0	0
			703	458	116	127	2			

- Molecule 2 is water.

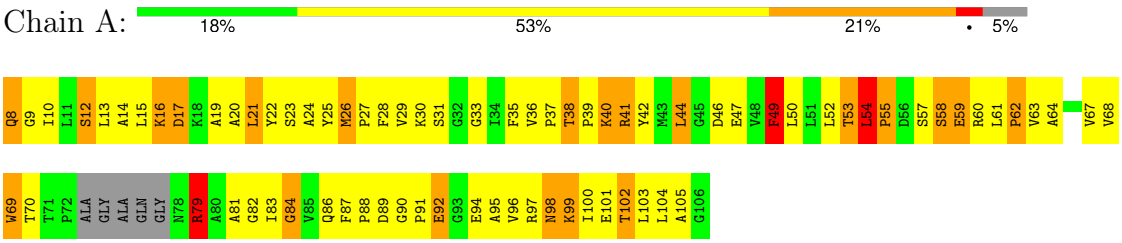
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	45	Total	O	0	0
			45	45		
2	B	44	Total	O	0	0
			44	44		
2	C	37	Total	O	0	0
			37	37		

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 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.

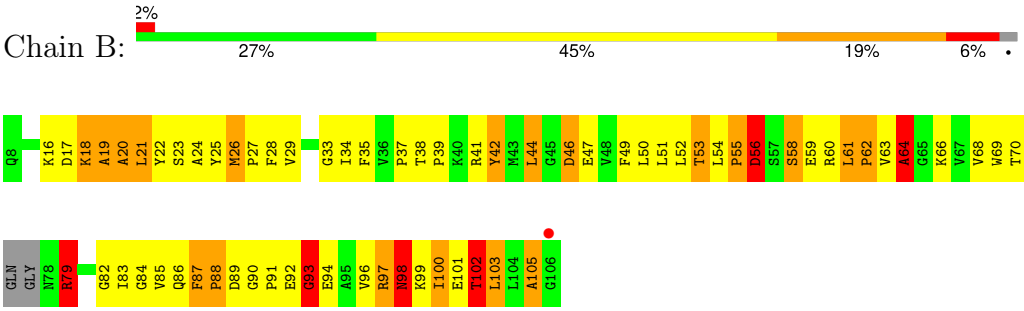
• Molecule 1: Type IV fimbriae assembly protein

Chain A:



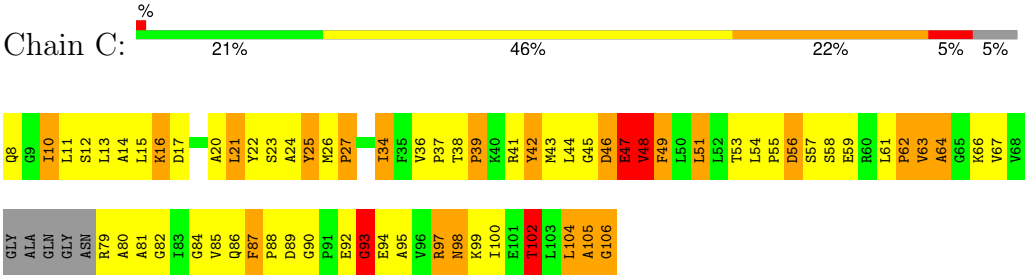
• Molecule 1: Type IV fimbriae assembly protein

Chain B:



• Molecule 1: Type IV fimbriae assembly protein

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	87.90Å 50.96Å 92.75Å 90.00° 90.21° 90.00°	Depositor
Resolution (Å)	25.48 – 2.09 25.48 – 2.09	Depositor EDS
% Data completeness (in resolution range)	88.6 (25.48-2.09) 95.4 (25.48-2.09)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.22	Depositor
$< I/\sigma(I) >$ [1]	7.18 (at 2.10Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.277 , 0.278 0.276 , 0.305	Depositor DCC
R_{free} test set	1212 reflections (5.30%)	wwPDB-VP
Wilson B-factor (Å^2)	52.9	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 65.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.028 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.026 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.447 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.438 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.021 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	2263	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% 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	2.55	28/723 (3.9%)	3.41	121/976 (12.4%)
1	B	2.59	29/737 (3.9%)	3.29	114/995 (11.5%)
1	C	2.76	39/716 (5.4%)	3.23	93/967 (9.6%)
All	All	2.63	96/2176 (4.4%)	3.31	328/2938 (11.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	6
1	C	0	5
All	All	0	17

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	106	GLY	C-OXT	22.45	1.68	1.23
1	B	50	LEU	CA-C	-15.02	1.34	1.52
1	C	82	GLY	C-O	-10.79	1.09	1.23
1	C	17	ASP	C-O	-9.32	1.12	1.23
1	C	14	ALA	CA-C	-9.30	1.41	1.52
1	C	25	TYR	C-O	-8.80	1.13	1.23
1	B	66	LYS	C-N	-8.35	1.25	1.33
1	C	42	TYR	C-O	-8.25	1.13	1.23
1	C	54	LEU	C-N	8.14	1.43	1.33
1	C	93	GLY	C-O	-8.06	1.14	1.23
1	C	71	THR	C-O	-8.03	1.16	1.24
1	C	61	LEU	C-N	7.90	1.43	1.33
1	B	61	LEU	C-N	7.83	1.43	1.33
1	C	72	PRO	N-CD	7.81	1.58	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	SER	C-O	-7.78	1.13	1.24
1	C	58	SER	C-O	-7.78	1.13	1.24
1	B	54	LEU	C-N	7.75	1.43	1.33
1	B	27	PRO	C-N	-7.44	1.23	1.33
1	A	42	TYR	C-O	-7.32	1.14	1.23
1	B	38	THR	C-N	7.30	1.39	1.33
1	A	84	GLY	C-O	-7.26	1.14	1.23
1	A	61	LEU	C-N	7.14	1.42	1.33
1	B	16	LYS	C-O	-7.09	1.15	1.24
1	B	21	LEU	C-N	-7.01	1.24	1.33
1	C	23	SER	N-CA	-6.82	1.38	1.46
1	A	67	VAL	C-N	-6.70	1.26	1.33
1	C	36	VAL	C-N	6.57	1.42	1.33
1	B	62	PRO	C-N	-6.49	1.25	1.33
1	C	66	LYS	C-N	-6.49	1.25	1.33
1	A	38	THR	C-N	6.41	1.40	1.34
1	C	97	ARG	C-O	-6.35	1.16	1.24
1	C	90	GLY	C-N	6.34	1.42	1.33
1	B	61	LEU	C-O	-6.33	1.17	1.24
1	A	35	PHE	C-N	-6.26	1.26	1.33
1	C	13	LEU	C-N	-6.24	1.24	1.33
1	A	19	ALA	C-O	-6.23	1.16	1.24
1	C	37	PRO	N-CD	-6.22	1.39	1.47
1	B	33	GLY	C-N	-6.18	1.26	1.33
1	C	38	THR	C-N	6.18	1.38	1.33
1	B	71	THR	C-O	-6.18	1.15	1.24
1	A	88	PRO	N-CD	-6.15	1.39	1.47
1	A	33	GLY	C-N	-6.06	1.26	1.33
1	B	103	LEU	C-N	-6.04	1.24	1.33
1	B	19	ALA	C-N	-5.99	1.25	1.33
1	B	18	LYS	C-N	-5.96	1.26	1.33
1	A	91	PRO	C-N	-5.95	1.26	1.34
1	A	26	MSE	C-O	-5.95	1.17	1.24
1	B	96	VAL	C-N	-5.93	1.25	1.33
1	C	92	GLU	C-N	-5.93	1.27	1.33
1	A	101	GLU	C-N	-5.92	1.26	1.33
1	A	28	PHE	C-N	-5.91	1.26	1.33
1	B	39	PRO	C-N	-5.88	1.25	1.33
1	A	99	LYS	C-N	-5.77	1.26	1.33
1	C	36	VAL	C-O	-5.73	1.17	1.24
1	C	51	LEU	CA-C	-5.68	1.45	1.52
1	A	81	ALA	C-N	-5.64	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	PRO	N-CD	-5.62	1.39	1.47
1	B	34	ILE	CA-CB	-5.61	1.48	1.55
1	C	89	ASP	C-N	-5.58	1.25	1.33
1	A	39	PRO	C-N	-5.54	1.26	1.33
1	B	87	PHE	C-O	-5.52	1.17	1.24
1	C	84	GLY	C-N	-5.51	1.25	1.33
1	A	38	THR	C-O	-5.48	1.17	1.24
1	C	97	ARG	C-N	-5.47	1.27	1.33
1	C	86	GLN	C-N	-5.46	1.25	1.33
1	C	87	PHE	C-N	5.46	1.40	1.33
1	B	37	PRO	N-CD	-5.44	1.40	1.47
1	A	61	LEU	C-O	-5.44	1.17	1.24
1	B	64	ALA	C-N	-5.43	1.28	1.33
1	A	91	PRO	N-CD	5.39	1.55	1.47
1	C	27	PRO	N-CD	-5.39	1.40	1.47
1	B	87	PHE	C-N	5.37	1.40	1.33
1	B	39	PRO	N-CD	-5.35	1.40	1.47
1	C	61	LEU	C-O	-5.33	1.17	1.24
1	C	22	TYR	C-N	-5.32	1.26	1.33
1	A	95	ALA	C-N	-5.29	1.27	1.33
1	C	87	PHE	C-O	-5.29	1.17	1.23
1	B	38	THR	C-O	-5.28	1.17	1.24
1	C	20	ALA	CA-CB	-5.26	1.45	1.53
1	A	14	ALA	C-N	-5.26	1.24	1.33
1	A	36	VAL	C-O	-5.25	1.17	1.24
1	A	27	PRO	N-CD	-5.25	1.40	1.47
1	A	68	VAL	N-CA	-5.25	1.41	1.46
1	A	10	ILE	C-N	-5.23	1.24	1.33
1	C	39	PRO	C-N	-5.22	1.26	1.33
1	A	36	VAL	C-N	5.21	1.40	1.33
1	B	84	GLY	C-N	-5.19	1.26	1.33
1	B	91	PRO	N-CD	-5.18	1.40	1.47
1	C	38	THR	C-O	-5.18	1.17	1.24
1	C	95	ALA	C-N	-5.17	1.27	1.33
1	B	20	ALA	C-O	-5.15	1.18	1.24
1	C	39	PRO	N-CA	-5.09	1.42	1.47
1	B	100	ILE	C-N	-5.04	1.27	1.33
1	B	62	PRO	N-CD	5.01	1.54	1.47
1	C	48	VAL	C-N	-5.01	1.26	1.33
1	C	11	LEU	C-N	-5.00	1.26	1.33

All (328) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	16	LYS	O-C-N	-21.15	98.04	122.15
1	B	16	LYS	CA-C-O	19.22	140.79	120.42
1	C	58	SER	O-C-N	-18.13	100.58	122.34
1	A	58	SER	O-C-N	-17.74	100.44	122.26
1	B	87	PHE	CA-C-O	16.81	136.33	120.02
1	B	87	PHE	CA-C-N	-15.29	104.89	120.03
1	B	87	PHE	C-N-CA	-15.29	104.89	120.03
1	C	64	ALA	O-C-N	-14.81	102.83	122.38
1	C	58	SER	CA-C-O	14.54	136.57	119.56
1	B	93	GLY	O-C-N	-14.30	104.11	122.70
1	A	31	SER	O-C-N	-13.62	107.31	121.88
1	C	93	GLY	O-C-N	-13.33	109.39	122.19
1	C	87	PHE	CA-C-N	-12.66	107.50	120.03
1	C	87	PHE	C-N-CA	-12.66	107.50	120.03
1	A	60	ARG	CA-C-N	12.31	137.99	121.74
1	A	60	ARG	C-N-CA	12.31	137.99	121.74
1	A	79	ARG	CD-NE-CZ	12.29	141.61	124.40
1	C	92	GLU	CA-C-N	12.06	133.09	119.94
1	C	92	GLU	C-N-CA	12.06	133.09	119.94
1	C	89	ASP	CA-CB-CG	11.83	124.43	112.60
1	B	55	PRO	O-C-N	-11.66	108.08	122.89
1	C	54	LEU	CA-C-N	-11.51	108.16	119.90
1	C	54	LEU	C-N-CA	-11.51	108.16	119.90
1	A	82	GLY	N-CA-C	11.35	125.20	110.45
1	B	54	LEU	CA-C-N	-11.06	108.61	119.90
1	B	54	LEU	C-N-CA	-11.06	108.61	119.90
1	A	87	PHE	O-C-N	-11.06	109.04	121.43
1	A	46	ASP	CA-CB-CG	10.96	123.56	112.60
1	A	38	THR	CA-C-N	-10.76	108.96	120.47
1	A	38	THR	C-N-CA	-10.76	108.96	120.47
1	B	46	ASP	CA-CB-CG	10.74	123.34	112.60
1	C	25	TYR	CA-C-O	10.68	133.12	121.16
1	C	38	THR	CA-C-N	-10.67	108.62	121.00
1	C	38	THR	C-N-CA	-10.67	108.62	121.00
1	B	88	PRO	CA-C-N	10.62	135.79	120.71
1	B	88	PRO	C-N-CA	10.62	135.79	120.71
1	A	81	ALA	CA-C-N	10.47	137.77	121.12
1	A	81	ALA	C-N-CA	10.47	137.77	121.12
1	A	54	LEU	CA-C-N	-10.46	106.77	119.84
1	A	54	LEU	C-N-CA	-10.46	106.77	119.84
1	B	46	ASP	CA-C-N	10.46	137.88	121.26
1	B	46	ASP	C-N-CA	10.46	137.88	121.26
1	A	19	ALA	CA-C-O	10.15	131.50	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	61	LEU	CA-C-N	-10.12	109.06	119.99
1	A	61	LEU	C-N-CA	-10.12	109.06	119.99
1	C	88	PRO	CA-C-N	9.96	134.87	120.82
1	C	88	PRO	C-N-CA	9.96	134.87	120.82
1	C	98	ASN	CA-CB-CG	9.94	122.53	112.60
1	B	55	PRO	CA-C-O	9.88	132.53	121.36
1	C	46	ASP	CA-CB-CG	9.84	122.44	112.60
1	C	61	LEU	CA-C-N	-9.77	109.44	119.99
1	C	61	LEU	C-N-CA	-9.77	109.44	119.99
1	B	59	GLU	CA-C-N	9.11	135.29	122.72
1	B	59	GLU	C-N-CA	9.11	135.29	122.72
1	A	95	ALA	CA-C-N	8.97	131.87	120.56
1	A	95	ALA	C-N-CA	8.97	131.87	120.56
1	B	83	ILE	CA-C-N	8.90	138.85	121.41
1	B	83	ILE	C-N-CA	8.90	138.85	121.41
1	A	31	SER	CA-C-O	8.88	133.33	118.94
1	B	86	GLN	CA-C-N	8.76	133.22	120.51
1	B	86	GLN	C-N-CA	8.76	133.22	120.51
1	A	89	ASP	CA-CB-CG	8.68	121.28	112.60
1	A	21	LEU	CA-C-N	8.66	132.25	120.38
1	A	21	LEU	C-N-CA	8.66	132.25	120.38
1	A	98	ASN	CA-CB-CG	8.64	121.24	112.60
1	A	59	GLU	CA-C-N	8.54	135.01	123.05
1	A	59	GLU	C-N-CA	8.54	135.01	123.05
1	A	91	PRO	CA-C-N	8.47	132.74	120.38
1	A	91	PRO	C-N-CA	8.47	132.74	120.38
1	A	19	ALA	O-C-N	-8.46	111.23	122.23
1	B	59	GLU	CB-CG-CD	8.46	126.97	112.60
1	C	87	PHE	CA-C-O	8.39	129.85	120.70
1	A	36	VAL	CA-C-N	-8.39	111.12	119.76
1	A	36	VAL	C-N-CA	-8.39	111.12	119.76
1	B	61	LEU	CA-C-O	8.33	127.26	119.59
1	B	87	PHE	O-C-N	-8.31	113.21	121.27
1	C	102	THR	O-C-N	-8.23	112.76	122.15
1	C	36	VAL	CA-C-N	-8.19	111.57	119.76
1	C	36	VAL	C-N-CA	-8.19	111.57	119.76
1	A	90	GLY	O-C-N	8.12	129.89	121.77
1	C	53	THR	CA-C-N	8.12	132.01	120.49
1	C	53	THR	C-N-CA	8.12	132.01	120.49
1	C	102	THR	CA-CB-OG1	8.08	121.72	109.60
1	C	64	ALA	CA-C-O	8.04	132.14	122.41
1	A	96	VAL	N-CA-CB	8.04	119.95	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	71	THR	O-C-N	8.03	128.10	121.44
1	C	56	ASP	CA-CB-CG	8.01	120.61	112.60
1	A	61	LEU	CA-C-O	7.99	124.49	119.29
1	A	23	SER	N-CA-C	7.92	121.01	111.82
1	B	61	LEU	CA-C-N	-7.89	111.46	119.99
1	B	61	LEU	C-N-CA	-7.89	111.46	119.99
1	B	98	ASN	CA-CB-CG	7.88	120.48	112.60
1	A	62	PRO	CA-N-CD	-7.87	100.98	112.00
1	C	41	ARG	NE-CZ-NH2	7.87	126.28	119.20
1	C	69	TRP	O-C-N	-7.86	112.14	122.59
1	A	97	ARG	CA-C-O	7.83	128.84	120.55
1	A	87	PHE	CA-CB-CG	7.82	121.62	113.80
1	A	12	SER	CA-C-N	7.70	133.60	122.44
1	A	12	SER	C-N-CA	7.70	133.60	122.44
1	C	72	PRO	CA-N-CD	-7.69	101.24	112.00
1	C	27	PRO	CA-C-N	7.68	136.38	121.18
1	C	27	PRO	C-N-CA	7.68	136.38	121.18
1	B	82	GLY	N-CA-C	7.65	121.56	110.63
1	A	79	ARG	NE-CZ-NH1	7.64	129.14	121.50
1	A	59	GLU	CB-CG-CD	7.63	125.56	112.60
1	A	16	LYS	N-CA-C	7.59	119.55	111.28
1	A	61	LEU	N-CA-CB	7.50	119.70	110.17
1	B	102	THR	CA-CB-OG1	7.50	120.84	109.60
1	B	21	LEU	N-CA-CB	7.48	121.19	109.82
1	C	59	GLU	CA-C-N	7.43	133.46	123.05
1	C	59	GLU	C-N-CA	7.43	133.46	123.05
1	A	49	PHE	CA-CB-CG	7.41	121.21	113.80
1	A	46	ASP	CA-C-N	7.41	132.63	122.19
1	A	46	ASP	C-N-CA	7.41	132.63	122.19
1	B	90	GLY	CA-C-N	7.37	129.05	119.84
1	B	90	GLY	C-N-CA	7.37	129.05	119.84
1	C	46	ASP	CA-C-N	7.35	132.01	121.50
1	C	46	ASP	C-N-CA	7.35	132.01	121.50
1	A	38	THR	O-C-N	7.33	129.76	121.32
1	B	41	ARG	CA-C-N	7.33	134.97	122.37
1	B	41	ARG	C-N-CA	7.33	134.97	122.37
1	B	20	ALA	N-CA-CB	7.29	120.95	110.16
1	A	61	LEU	O-C-N	7.24	127.09	121.23
1	A	64	ALA	CA-C-N	-7.19	113.97	122.16
1	A	64	ALA	C-N-CA	-7.19	113.97	122.16
1	B	102	THR	CA-CB-CG2	7.18	122.71	110.50
1	B	87	PHE	N-CA-CB	7.18	120.30	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	102	THR	CA-CB-CG2	7.15	122.65	110.50
1	A	44	LEU	O-C-N	7.12	131.63	122.87
1	A	70	THR	O-C-N	-7.10	114.00	123.23
1	B	54	LEU	CA-C-O	7.10	127.47	120.23
1	C	17	ASP	O-C-N	-7.07	114.97	123.10
1	B	47	GLU	CA-C-N	-7.05	113.14	122.94
1	B	47	GLU	C-N-CA	-7.05	113.14	122.94
1	B	66	LYS	CA-C-N	7.00	133.46	121.63
1	B	66	LYS	C-N-CA	7.00	133.46	121.63
1	B	105	ALA	CA-C-N	6.99	134.29	121.70
1	B	105	ALA	C-N-CA	6.99	134.29	121.70
1	A	98	ASN	N-CA-CB	6.99	120.62	110.20
1	C	14	ALA	CA-C-O	6.99	128.01	120.32
1	A	21	LEU	N-CA-CB	6.95	120.39	109.82
1	B	93	GLY	CA-C-O	6.94	132.65	120.57
1	B	61	LEU	O-C-N	6.93	129.02	121.12
1	C	63	VAL	CA-CB-CG2	6.92	122.16	110.40
1	A	70	THR	CA-C-O	6.90	128.15	120.70
1	C	93	GLY	CA-C-O	6.88	128.61	120.90
1	A	41	ARG	NE-CZ-NH1	-6.82	114.68	121.50
1	B	89	ASP	CA-CB-CG	6.81	119.41	112.60
1	B	24	ALA	CA-C-N	6.79	130.40	120.82
1	B	24	ALA	C-N-CA	6.79	130.40	120.82
1	C	89	ASP	N-CA-CB	6.77	120.05	109.69
1	B	62	PRO	CA-N-CD	-6.75	102.55	112.00
1	B	38	THR	CA-C-N	-6.75	113.25	120.94
1	B	38	THR	C-N-CA	-6.75	113.25	120.94
1	B	97	ARG	CA-C-O	6.72	127.62	120.70
1	A	86	GLN	CA-C-N	6.72	130.03	120.49
1	A	86	GLN	C-N-CA	6.72	130.03	120.49
1	A	90	GLY	CA-C-N	-6.71	111.45	119.84
1	A	90	GLY	C-N-CA	-6.71	111.45	119.84
1	A	13	LEU	N-CA-C	6.70	119.39	107.80
1	C	63	VAL	CA-CB-CG1	6.69	121.77	110.40
1	A	12	SER	N-CA-C	6.67	121.17	109.96
1	B	38	THR	O-C-N	6.65	128.97	121.32
1	B	34	ILE	CA-C-N	6.59	131.54	122.77
1	B	34	ILE	C-N-CA	6.59	131.54	122.77
1	B	49	PHE	CA-CB-CG	6.56	120.36	113.80
1	C	21	LEU	N-CA-CB	6.52	119.46	110.01
1	A	63	VAL	CA-C-N	6.49	131.57	122.41
1	A	63	VAL	C-N-CA	6.49	131.57	122.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	87	PHE	CA-CB-CG	6.49	120.29	113.80
1	A	58	SER	CA-C-O	6.49	127.61	119.95
1	C	55	PRO	CA-N-CD	-6.47	102.95	112.00
1	A	8	GLN	OE1-CD-NE2	-6.43	116.17	122.60
1	C	90	GLY	O-C-N	6.42	128.19	121.77
1	C	37	PRO	CA-C-N	6.42	137.45	121.80
1	C	37	PRO	C-N-CA	6.42	137.45	121.80
1	C	17	ASP	CA-CB-CG	6.38	118.98	112.60
1	C	36	VAL	O-C-N	6.38	128.37	121.10
1	A	20	ALA	N-CA-C	6.36	118.21	111.28
1	C	61	LEU	CA-C-O	6.33	124.68	119.36
1	B	17	ASP	CA-CB-CG	6.31	118.91	112.60
1	B	41	ARG	NE-CZ-NH2	6.31	124.88	119.20
1	B	26	MSE	CA-C-N	6.30	125.99	119.56
1	B	26	MSE	C-N-CA	6.30	125.99	119.56
1	A	87	PHE	CA-C-O	6.24	126.99	120.25
1	C	20	ALA	N-CA-CB	6.21	119.35	110.16
1	B	47	GLU	CA-C-O	6.18	127.47	120.80
1	A	102	THR	N-CA-CB	6.15	119.16	110.12
1	A	9	GLY	N-CA-C	6.14	120.64	112.65
1	B	47	GLU	CA-CB-CG	6.11	126.32	114.10
1	C	102	THR	CB-CA-C	6.10	121.22	110.85
1	B	79	ARG	CA-C-N	6.09	130.51	120.94
1	B	79	ARG	C-N-CA	6.09	130.51	120.94
1	A	91	PRO	CA-N-CD	-6.09	103.48	112.00
1	A	61	LEU	C-N-CD	6.08	149.95	125.00
1	A	41	ARG	NE-CZ-NH2	6.07	124.67	119.20
1	A	24	ALA	N-CA-CB	6.07	119.15	110.16
1	B	23	SER	CB-CA-C	6.07	121.80	110.70
1	C	14	ALA	O-C-N	-6.05	116.13	123.27
1	B	25	TYR	N-CA-CB	6.05	118.95	109.69
1	B	70	THR	CA-CB-OG1	6.01	118.61	109.60
1	B	52	LEU	CA-C-N	6.01	130.65	122.84
1	B	52	LEU	C-N-CA	6.01	130.65	122.84
1	C	56	ASP	CA-C-O	6.01	129.10	120.51
1	A	55	PRO	CA-N-CD	-6.00	103.61	112.00
1	B	56	ASP	CA-C-O	5.99	128.57	121.08
1	B	21	LEU	CA-C-N	5.99	128.31	120.28
1	B	21	LEU	C-N-CA	5.99	128.31	120.28
1	B	60	ARG	O-C-N	-5.98	116.51	123.27
1	A	102	THR	CA-CB-OG1	5.97	118.56	109.60
1	A	54	LEU	C-N-CD	5.96	149.43	125.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	25	TYR	N-CA-CB	5.96	118.80	109.69
1	B	92	GLU	CB-CG-CD	5.95	122.71	112.60
1	B	37	PRO	CA-C-O	-5.91	114.91	121.23
1	C	38	THR	O-C-N	5.91	128.11	121.32
1	C	63	VAL	N-CA-CB	5.89	119.83	111.82
1	C	57	SER	O-C-N	5.87	129.85	123.10
1	B	58	SER	CA-C-N	5.87	131.44	122.93
1	B	58	SER	C-N-CA	5.87	131.44	122.93
1	A	68	VAL	CB-CA-C	5.85	116.94	110.62
1	B	70	THR	CA-C-O	-5.85	114.61	121.46
1	B	24	ALA	N-CA-C	5.83	117.72	111.36
1	C	54	LEU	C-N-CD	5.83	148.89	125.00
1	A	97	ARG	CA-CB-CG	5.82	125.74	114.10
1	B	47	GLU	N-CA-CB	5.82	118.83	109.28
1	B	53	THR	N-CA-C	5.81	118.14	108.20
1	C	12	SER	N-CA-C	5.81	119.15	110.14
1	A	92	GLU	CB-CG-CD	5.79	122.44	112.60
1	B	16	LYS	N-CA-C	5.79	117.67	111.36
1	B	55	PRO	CA-N-CD	-5.77	103.93	112.00
1	A	17	ASP	CA-C-O	-5.76	115.25	121.36
1	B	44	LEU	CA-C-N	5.76	131.56	122.51
1	B	44	LEU	C-N-CA	5.76	131.56	122.51
1	B	38	THR	CA-CB-OG1	5.76	118.24	109.60
1	A	63	VAL	CA-CB-CG2	5.75	120.17	110.40
1	C	97	ARG	NE-CZ-NH1	-5.74	115.76	121.50
1	B	23	SER	CA-C-N	5.74	128.43	120.29
1	B	23	SER	C-N-CA	5.74	128.43	120.29
1	A	92	GLU	CA-C-N	5.72	132.62	121.41
1	A	92	GLU	C-N-CA	5.72	132.62	121.41
1	A	104	LEU	CA-C-N	5.72	129.48	121.02
1	A	104	LEU	C-N-CA	5.72	129.48	121.02
1	B	102	THR	CB-CA-C	5.72	120.28	110.79
1	A	28	PHE	CA-C-N	5.72	129.80	121.80
1	A	28	PHE	C-N-CA	5.72	129.80	121.80
1	B	46	ASP	N-CA-CB	5.67	118.37	109.69
1	C	38	THR	CA-CB-OG1	5.67	118.10	109.60
1	B	105	ALA	O-C-N	5.66	128.60	122.15
1	B	60	ARG	CA-C-N	5.65	132.11	122.06
1	B	60	ARG	C-N-CA	5.65	132.11	122.06
1	A	9	GLY	CA-C-N	-5.62	114.87	122.91
1	A	9	GLY	C-N-CA	-5.62	114.87	122.91
1	C	104	LEU	CA-C-N	5.61	132.26	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	104	LEU	C-N-CA	5.61	132.26	121.54
1	C	59	GLU	CA-CB-CG	5.59	125.29	114.10
1	A	104	LEU	CA-C-O	5.58	125.89	119.35
1	B	27	PRO	CA-C-N	5.55	129.99	120.72
1	B	27	PRO	C-N-CA	5.55	129.99	120.72
1	C	24	ALA	N-CA-CB	5.55	118.85	110.30
1	A	69	TRP	CE2-CD2-CE3	5.55	124.35	118.80
1	B	53	THR	CA-C-N	5.55	137.06	120.69
1	B	53	THR	C-N-CA	5.55	137.06	120.69
1	C	38	THR	N-CA-CB	5.54	120.24	110.37
1	C	55	PRO	CA-C-O	5.54	127.62	121.36
1	A	44	LEU	CA-C-O	-5.53	115.11	121.19
1	A	84	GLY	CA-C-N	5.49	129.92	122.90
1	A	84	GLY	C-N-CA	5.49	129.92	122.90
1	C	54	LEU	N-CA-C	5.48	116.79	109.83
1	A	44	LEU	CA-C-N	5.48	132.63	121.78
1	A	44	LEU	C-N-CA	5.48	132.63	121.78
1	B	90	GLY	O-C-N	5.47	127.24	121.77
1	B	54	LEU	C-N-CD	5.46	147.39	125.00
1	B	99	LYS	N-CA-CB	5.45	118.13	110.12
1	A	22	TYR	N-CA-CB	5.45	118.23	110.06
1	A	92	GLU	CA-CB-CG	5.44	124.99	114.10
1	A	100	ILE	CB-CG1-CD1	5.44	125.23	113.80
1	B	24	ALA	N-CA-CB	5.44	118.21	110.16
1	B	17	ASP	N-CA-C	5.43	117.05	108.96
1	A	81	ALA	CA-C-O	-5.40	115.11	121.16
1	C	36	VAL	CA-CB-CG2	5.36	119.51	110.40
1	A	54	LEU	CA-C-O	5.34	125.68	120.23
1	C	98	ASN	OD1-CG-ND2	-5.34	117.25	122.60
1	A	67	VAL	CA-CB-CG2	5.33	119.46	110.40
1	B	41	ARG	N-CA-CB	5.32	119.26	110.69
1	C	81	ALA	CA-C-O	-5.29	115.94	121.55
1	C	62	PRO	CA-C-N	5.27	130.46	122.98
1	C	62	PRO	C-N-CA	5.27	130.46	122.98
1	B	59	GLU	CA-C-O	-5.26	115.13	120.71
1	A	83	ILE	CA-CB-CG1	5.25	119.33	110.40
1	B	63	VAL	CA-CB-CG2	5.25	119.33	110.40
1	C	97	ARG	NH1-CZ-NH2	5.25	126.12	119.30
1	C	105	ALA	CA-C-O	5.24	128.00	120.51
1	A	10	ILE	CA-CB-CG2	5.24	119.40	110.50
1	A	21	LEU	CA-C-O	-5.23	115.32	121.07
1	B	53	THR	OG1-CB-CG2	5.23	119.75	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	99	LYS	N-CA-CB	5.22	117.72	109.94
1	B	85	VAL	CA-CB-CG2	5.21	119.25	110.40
1	A	40	LYS	CA-C-N	5.21	130.34	123.05
1	A	40	LYS	C-N-CA	5.21	130.34	123.05
1	C	16	LYS	N-CA-C	5.19	117.61	111.33
1	A	17	ASP	CA-C-N	5.18	129.38	120.72
1	A	17	ASP	C-N-CA	5.18	129.38	120.72
1	B	28	PHE	N-CA-C	5.18	118.86	112.54
1	B	35	PHE	CA-CB-CG	-5.17	108.62	113.80
1	C	53	THR	CA-CB-CG2	5.17	119.29	110.50
1	A	55	PRO	CA-C-N	-5.16	115.57	123.47
1	A	55	PRO	C-N-CA	-5.16	115.57	123.47
1	B	22	TYR	N-CA-CB	5.15	117.69	110.12
1	C	49	PHE	CA-CB-CG	5.14	118.94	113.80
1	A	68	VAL	CA-C-O	5.13	123.60	118.98
1	A	64	ALA	O-C-N	-5.12	116.77	122.55
1	C	8	GLN	CA-C-N	5.11	132.79	120.99
1	C	8	GLN	C-N-CA	5.11	132.79	120.99
1	B	61	LEU	C-N-CD	5.10	145.92	125.00
1	A	89	ASP	N-CA-CB	5.10	118.04	110.29
1	B	42	TYR	CA-CB-CG	5.09	123.06	113.90
1	C	85	VAL	N-CA-CB	5.08	118.08	111.67
1	C	47	GLU	CB-CG-CD	5.07	121.22	112.60
1	A	96	VAL	CA-C-N	5.06	127.06	120.28
1	A	96	VAL	C-N-CA	5.06	127.06	120.28
1	C	70	THR	CA-C-N	5.05	128.38	122.52
1	C	70	THR	C-N-CA	5.05	128.38	122.52
1	C	92	GLU	N-CA-C	5.04	116.78	111.28
1	A	94	GLU	N-CA-C	5.03	117.50	111.71
1	B	29	VAL	CA-CB-CG2	5.02	118.94	110.40
1	A	97	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	C	85	VAL	CA-CB-CG1	5.01	118.91	110.40
1	C	82	GLY	N-CA-C	5.00	117.19	110.43

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	ALA	Mainchain
1	A	38	THR	Mainchain
1	A	49	PHE	Sidechain
1	A	58	SER	Mainchain

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Mol	Chain	Res	Type	Group
1	A	84	GLY	Mainchain
1	A	92	GLU	Mainchain
1	B	101	GLU	Mainchain
1	B	105	ALA	Mainchain
1	B	46	ASP	Mainchain
1	B	64	ALA	Mainchain
1	B	79	ARG	Sidechain
1	B	93	GLY	Mainchain
1	C	10	ILE	Mainchain
1	C	39	PRO	Mainchain
1	C	48	VAL	Mainchain
1	C	64	ALA	Mainchain
1	C	93	GLY	Mainchain

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	710	0	732	16	3
1	B	724	0	745	19	1
1	C	703	0	727	27	3
2	A	45	0	0	9	0
2	B	44	0	0	5	0
2	C	37	0	0	6	0
All	All	2263	0	2204	58	4

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 (58) 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:C:106:GLY:C	1:C:106:GLY:OXT	1.68	1.33
1:B:26:MSE:HG2	2:B:350:HOH:O	1.08	1.22
1:A:26:MSE:HG2	2:A:203:HOH:O	1.05	1.18
1:C:26:MSE:HG2	2:C:425:HOH:O	1.00	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LYS:HD3	2:A:654:HOH:O	1.44	1.14
1:B:42:TYR:OH	2:B:638:HOH:O	1.78	1.00
1:C:79:ARG:NH2	2:C:628:HOH:O	1.97	0.95
1:A:16:LYS:HB3	2:A:492:HOH:O	1.74	0.86
1:C:47:GLU:HG3	2:C:646:HOH:O	1.79	0.81
1:B:98:ASN:O	1:B:102:THR:HG23	1.80	0.81
1:C:94:GLU:CD	1:C:97:ARG:HH11	1.92	0.78
1:B:58:SER:O	1:C:43:MSE:HG2	1.86	0.75
1:C:79:ARG:HG2	1:C:80:ALA:H	1.55	0.71
1:B:97:ARG:NH2	2:B:446:HOH:O	2.27	0.67
1:C:16:LYS:HE2	2:C:500:HOH:O	1.94	0.67
1:C:21:LEU:HD21	1:C:100:ILE:HG23	1.75	0.67
1:C:98:ASN:O	1:C:102:THR:HG23	1.96	0.65
1:C:94:GLU:OE2	1:C:97:ARG:NH1	2.31	0.63
1:A:15:LEU:HD13	1:A:21:LEU:HA	1.82	0.61
1:B:58:SER:O	1:C:43:MSE:HE3	2.01	0.61
1:C:25:TYR:O	1:C:27:PRO:HD3	2.01	0.61
1:B:18:LYS:HE2	1:B:103:LEU:O	2.01	0.60
1:A:47:GLU:HG2	2:A:653:HOH:O	2.00	0.59
1:A:57:SER:HB3	2:A:635:HOH:O	2.02	0.59
1:A:49:PHE:HE1	1:B:19:ALA:HA	1.69	0.57
1:B:20:ALA:O	2:B:403:HOH:O	2.18	0.56
1:A:40:LYS:CD	2:A:654:HOH:O	2.23	0.55
1:B:21:LEU:HD21	1:B:100:ILE:HG23	1.87	0.54
1:C:79:ARG:CG	1:C:80:ALA:H	2.21	0.54
1:A:53:THR:OG1	2:A:204:HOH:O	2.18	0.54
1:B:55:PRO:O	1:B:56:ASP:C	2.49	0.52
1:A:54:LEU:O	1:A:55:PRO:C	2.51	0.52
1:B:93:GLY:O	1:B:94:GLU:C	2.53	0.52
1:B:94:GLU:HG3	1:B:97:ARG:HH11	1.76	0.51
1:B:64:ALA:O	1:B:88:PRO:HD3	2.11	0.50
1:C:79:ARG:HG2	1:C:80:ALA:N	2.24	0.49
1:C:93:GLY:O	1:C:94:GLU:C	2.53	0.48
1:C:72:PRO:O	1:C:73:ALA:CB	2.62	0.48
1:C:62:PRO:HD2	2:C:631:HOH:O	2.13	0.47
1:A:79:ARG:NH2	2:A:449:HOH:O	2.47	0.47
1:C:42:TYR:CE2	1:C:48:VAL:HG22	2.51	0.46
1:C:48:VAL:HG23	1:C:67:VAL:HG23	1.98	0.46
1:B:62:PRO:HD2	2:B:420:HOH:O	2.15	0.45
1:B:94:GLU:HG3	1:B:97:ARG:NH1	2.30	0.45
1:B:72:PRO:O	1:B:73:ALA:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:PHE:O	1:B:88:PRO:C	2.53	0.45
1:A:62:PRO:HD2	2:A:618:HOH:O	2.18	0.44
1:C:34:ILE:HG22	1:C:87:PHE:HE1	1.81	0.44
1:A:17:ASP:C	1:A:55:PRO:HG3	2.43	0.43
1:A:41:ARG:HH11	1:A:41:ARG:HD2	1.48	0.43
1:C:10:ILE:HG12	1:C:49:PHE:CD2	2.53	0.43
1:C:15:LEU:HD13	1:C:21:LEU:HA	2.01	0.43
1:A:29:VAL:O	1:A:30:LYS:C	2.57	0.43
1:B:58:SER:C	1:C:43:MSE:HE3	2.44	0.42
1:C:51:LEU:HD12	1:C:51:LEU:HA	1.96	0.41
1:C:16:LYS:CE	2:C:500:HOH:O	2.63	0.41
1:A:98:ASN:O	1:A:99:LYS:C	2.64	0.40
1:C:45:GLY:O	1:C:46:ASP:C	2.62	0.40

All (4) 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:A:69:TRP:CZ2	1:C:69:TRP:NE1[3_555]	1.84	0.36
1:B:69:TRP:CZ2	1:B:69:TRP:CZ2[2_656]	2.08	0.12
1:A:69:TRP:CZ2	1:C:69:TRP:CE2[3_555]	2.11	0.09
1:A:69:TRP:CH2	1:C:69:TRP:NE1[3_555]	2.16	0.04

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	90/99 (91%)	87 (97%)	2 (2%)	1 (1%)	12 8
1	B	93/99 (94%)	88 (95%)	5 (5%)	0	100 100
1	C	90/99 (91%)	82 (91%)	5 (6%)	3 (3%)	3 1
All	All	273/297 (92%)	257 (94%)	12 (4%)	4 (2%)	8 5

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	ARG
1	C	105	ALA
1	C	34	ILE
1	C	72	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	75/74 (101%)	64 (85%)	11 (15%)	2 1
1	B	75/74 (101%)	66 (88%)	9 (12%)	4 2
1	C	73/74 (99%)	67 (92%)	6 (8%)	9 7
All	All	223/222 (100%)	197 (88%)	26 (12%)	4 2

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	12	SER
1	A	44	LEU
1	A	50	LEU
1	A	52	LEU
1	A	53	THR
1	A	54	LEU
1	A	59	GLU
1	A	79	ARG
1	A	102	THR
1	A	103	LEU
1	B	44	LEU
1	B	51	LEU
1	B	53	THR
1	B	56	ASP
1	B	61	LEU
1	B	68	VAL

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Mol	Chain	Res	Type
1	B	79	ARG
1	B	98	ASN
1	B	102	THR
1	C	44	LEU
1	C	47	GLU
1	C	56	ASP
1	C	63	VAL
1	C	102	THR
1	C	104	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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

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	92/99 (92%)	-0.35	0 100 100	38, 53, 75, 83	0
1	B	95/99 (95%)	-0.23	2 (2%) 63 65	39, 56, 81, 86	0
1	C	92/99 (92%)	-0.24	1 (1%) 77 78	39, 55, 75, 86	0
All	All	279/297 (93%)	-0.27	3 (1%) 77 78	38, 55, 80, 86	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	73	ALA	3.1
1	B	106	GLY	2.4
1	B	73	ALA	2.0

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 monosaccharides 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.