



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:54 AM UTC

PDB ID : 1S4I / pdb_00001s4i
Title : Crystal structure of a SOD-like protein from Bacillus subtilis
Authors : Banci, L.; Bertini, I.; Calderone, V.; Cramaro, F.; Del Conte, R.; Fantoni, A.; Mangani, S.; Quattrone, A.; Viezzoli, M.S.
Deposited on : 2004-01-16
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

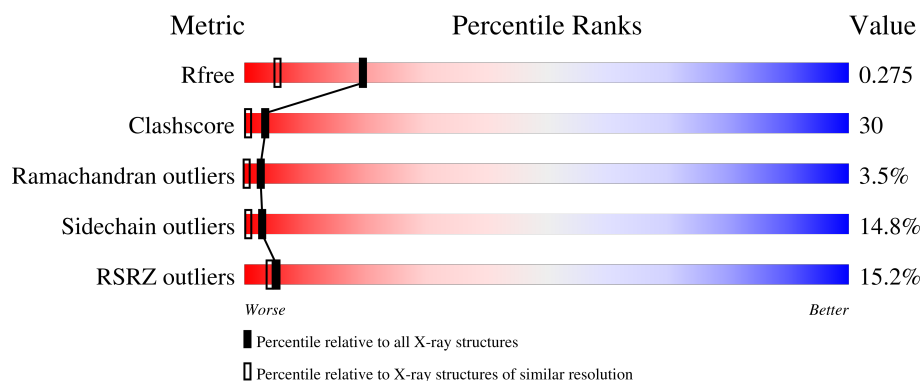
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 $\leq 5\%$. 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	175	
1	B	175	
1	C	175	
1	D	175	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4920 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 superoxide dismutase-like protein yojM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	152	Total	C	N	O	S	0	0	0
			1133	704	201	224	4			
1	A	151	Total	C	N	O	S	0	0	0
			1129	702	200	223	4			
1	C	151	Total	C	N	O	S	0	0	0
			1129	702	200	223	4			
1	D	151	Total	C	N	O	S	0	0	0
			1129	702	200	223	4			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		

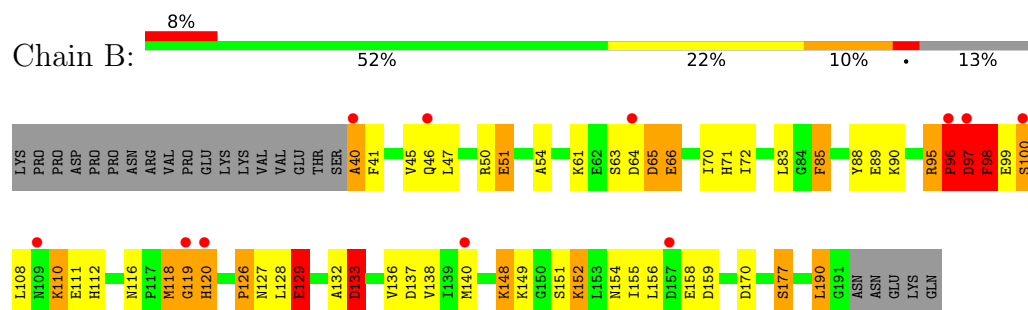
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	117	Total 117	O 117	0	0
4	A	93	Total 93	O 93	0	0
4	C	83	Total 83	O 83	0	0
4	D	97	Total 97	O 97	0	0

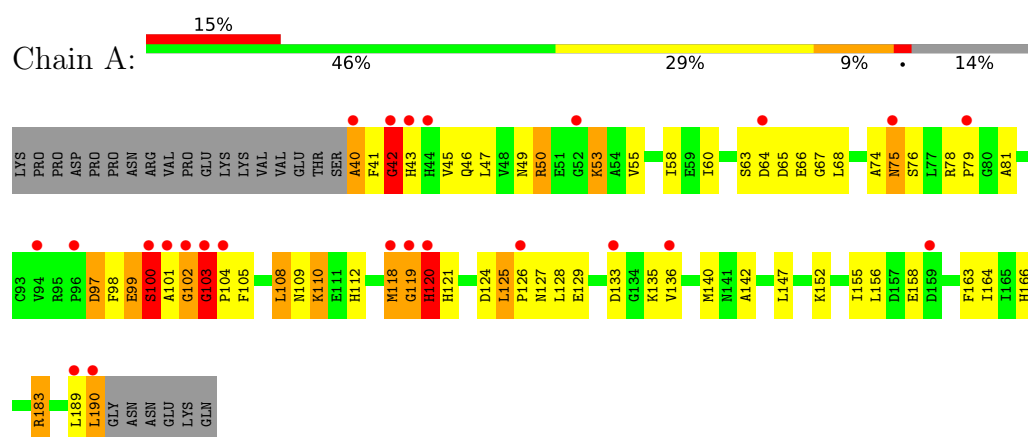
3 Residue-property plots [i](#)

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 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.

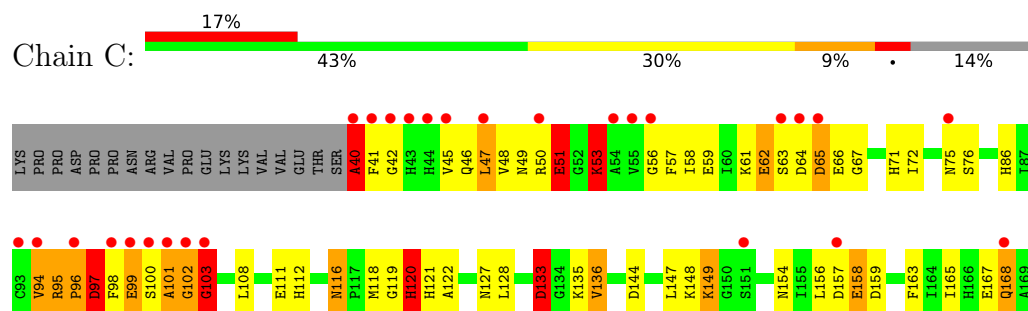
- Molecule 1: superoxide dismutase-like protein yojM

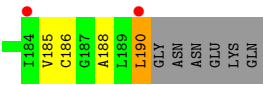


- Molecule 1: superoxide dismutase-like protein yojM

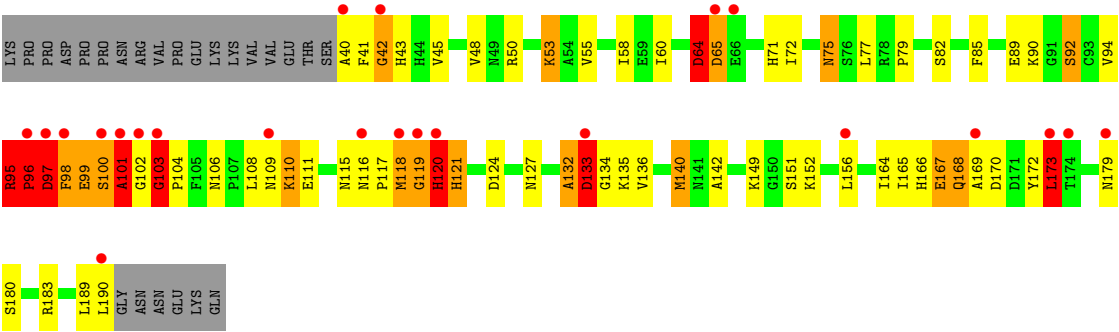


- Molecule 1: superoxide dismutase-like protein yojM





● Molecule 1: superoxide dismutase-like protein yojM



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	38.23Å 61.11Å 64.92Å 84.35° 76.02° 90.42°	Depositor
Resolution (Å)	37.01 – 1.80 37.01 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.01-1.80) 94.6 (37.01-1.80)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.54 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.221 , 0.258 0.250 , 0.275	Depositor DCC
R_{free} test set	8080 reflections (8.35%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4920	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.54	5/1153 (0.4%)	1.64	20/1558 (1.3%)
1	B	1.78	13/1157 (1.1%)	2.06	30/1563 (1.9%)
1	C	1.48	6/1153 (0.5%)	1.66	17/1558 (1.1%)
1	D	1.75	15/1153 (1.3%)	2.14	58/1558 (3.7%)
All	All	1.64	39/4616 (0.8%)	1.89	125/6237 (2.0%)

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	7
1	B	0	7
1	C	0	4
1	D	1	10
All	All	2	28

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	120	HIS	C-N	18.20	1.59	1.33
1	B	97	ASP	C-N	-15.27	1.12	1.33
1	B	96	PRO	C-N	-15.27	1.12	1.33
1	D	65	ASP	C-N	-13.49	1.14	1.33
1	D	65	ASP	C-O	12.04	1.39	1.23
1	D	97	ASP	C-N	11.52	1.49	1.33
1	B	97	ASP	C-O	11.17	1.38	1.24
1	D	96	PRO	N-CD	10.68	1.62	1.47
1	D	102	GLY	C-N	-10.55	1.17	1.33
1	D	102	GLY	CA-C	-9.32	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	GLY	N-CA	-8.34	1.36	1.44
1	D	102	GLY	N-CA	8.22	1.52	1.45
1	C	99	GLU	C-O	-7.95	1.14	1.24
1	A	183	ARG	CA-C	-7.63	1.43	1.52
1	C	41	PHE	C-N	7.55	1.44	1.33
1	D	95	ARG	N-CA	-7.22	1.35	1.46
1	D	142	ALA	CA-C	7.04	1.61	1.52
1	D	104	PRO	N-CD	6.85	1.57	1.47
1	C	163	PHE	CA-C	-6.72	1.44	1.52
1	B	96	PRO	C-O	6.71	1.36	1.23
1	B	54	ALA	CA-CB	-6.29	1.43	1.53
1	D	95	ARG	C-O	6.23	1.32	1.24
1	C	41	PHE	N-CA	-6.19	1.38	1.46
1	B	85	PHE	C-O	-5.99	1.16	1.23
1	D	136	VAL	C-O	5.97	1.30	1.24
1	B	70	ILE	CA-C	5.96	1.60	1.52
1	B	95	ARG	C-N	5.94	1.45	1.34
1	D	142	ALA	C-O	-5.92	1.17	1.24
1	C	188	ALA	CA-C	-5.92	1.45	1.52
1	B	155	ILE	CA-CB	5.75	1.62	1.54
1	D	173	LEU	N-CA	5.63	1.53	1.46
1	B	118	MET	SD-CE	5.53	1.93	1.79
1	A	169	ALA	CA-C	-5.52	1.45	1.52
1	B	133	ASP	CA-CB	5.32	1.62	1.53
1	A	76	SER	CA-C	-5.18	1.46	1.53
1	C	186	CYS	CA-C	-5.15	1.46	1.52
1	D	42	GLY	C-O	5.14	1.30	1.23
1	B	71	HIS	CA-C	5.11	1.59	1.52
1	B	126	PRO	CA-CB	-5.03	1.46	1.53

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	96	PRO	CA-C-N	25.17	169.61	121.54
1	B	96	PRO	C-N-CA	25.17	169.61	121.54
1	B	97	ASP	O-C-N	-21.93	93.42	122.59
1	D	65	ASP	CA-C-O	-20.26	98.99	121.88
1	D	99	GLU	CA-C-N	15.63	146.30	122.23
1	D	99	GLU	C-N-CA	15.63	146.30	122.23
1	D	102	GLY	CA-C-O	13.32	132.09	122.37
1	D	102	GLY	O-C-N	-13.29	110.19	123.48
1	D	95	ARG	O-C-N	-12.82	106.58	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	97	ASP	CA-C-O	-12.04	103.30	120.51
1	C	41	PHE	O-C-N	-11.56	108.80	123.02
1	D	101	ALA	CA-C-N	-11.30	107.48	122.63
1	D	101	ALA	C-N-CA	-11.30	107.48	122.63
1	D	104	PRO	CA-N-CD	-10.56	97.21	112.00
1	D	104	PRO	O-C-N	-10.27	111.20	123.01
1	C	119	GLY	N-CA-C	9.97	126.57	112.82
1	D	96	PRO	CA-N-CD	-9.84	97.72	111.50
1	C	103	GLY	CA-C-O	-9.79	107.52	121.52
1	B	41	PHE	N-CA-C	-9.45	93.50	108.90
1	C	40	ALA	CA-C-N	9.39	135.34	121.72
1	C	40	ALA	C-N-CA	9.39	135.34	121.72
1	A	119	GLY	N-CA-C	8.96	126.74	112.58
1	A	41	PHE	N-CA-C	-8.91	95.82	110.17
1	D	97	ASP	CA-C-O	-8.80	110.02	119.08
1	A	118	MET	CA-C-O	8.55	129.56	119.56
1	B	96	PRO	CA-C-O	-8.46	99.89	120.20
1	C	102	GLY	CA-C-N	8.09	134.57	121.87
1	C	102	GLY	C-N-CA	8.09	134.57	121.87
1	A	104	PRO	N-CA-C	-8.01	98.65	111.38
1	D	98	PHE	O-C-N	-7.99	111.97	122.59
1	D	120	HIS	O-C-N	-7.88	112.11	122.59
1	D	101	ALA	CB-CA-C	7.78	122.17	110.50
1	D	71	HIS	N-CA-C	-7.61	94.52	107.99
1	C	75	ASN	CB-CA-C	-7.57	95.92	111.22
1	D	95	ARG	N-CA-CB	7.40	123.54	110.37
1	D	41	PHE	N-CA-C	-7.39	98.28	110.17
1	A	99	GLU	N-CA-C	-7.21	103.75	112.54
1	D	100	SER	O-C-N	-7.19	113.14	122.56
1	D	95	ARG	C-N-CD	7.10	136.21	120.60
1	D	95	ARG	CA-C-O	-7.00	110.57	120.16
1	D	104	PRO	N-CA-C	7.00	121.81	111.03
1	C	41	PHE	CA-CB-CG	6.93	120.73	113.80
1	D	100	SER	CA-C-N	6.83	134.00	121.70
1	D	100	SER	C-N-CA	6.83	134.00	121.70
1	B	98	PHE	O-C-N	-6.79	113.56	122.59
1	D	98	PHE	CA-C-O	6.64	130.00	120.51
1	B	103	GLY	CA-C-O	-6.62	112.06	121.52
1	D	132	ALA	CA-C-N	6.54	134.04	121.54
1	D	132	ALA	C-N-CA	6.54	134.04	121.54
1	D	42	GLY	N-CA-C	6.51	128.60	113.18
1	C	168	GLN	CB-CA-C	-6.50	97.46	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	138	VAL	CA-C-N	-6.45	115.19	123.19
1	B	138	VAL	C-N-CA	-6.45	115.19	123.19
1	A	120	HIS	CB-CA-C	6.41	123.18	110.42
1	D	96	PRO	CA-C-N	6.41	131.69	121.18
1	D	96	PRO	C-N-CA	6.41	131.69	121.18
1	D	104	PRO	N-CA-CB	6.33	108.97	103.27
1	A	119	GLY	CA-C-N	6.33	133.63	121.54
1	A	119	GLY	C-N-CA	6.33	133.63	121.54
1	A	109	ASN	N-CA-C	6.32	119.89	111.30
1	B	98	PHE	CA-CB-CG	6.29	120.09	113.80
1	D	119	GLY	CA-C-O	-6.24	114.52	121.94
1	D	101	ALA	O-C-N	-6.23	113.03	123.00
1	A	118	MET	N-CA-C	-6.22	105.26	112.92
1	B	137	ASP	CA-C-N	-6.21	113.87	122.69
1	B	137	ASP	C-N-CA	-6.21	113.87	122.69
1	D	103	GLY	CA-C-N	-6.19	113.15	119.83
1	D	103	GLY	C-N-CA	-6.19	113.15	119.83
1	C	116	ASN	N-CA-C	-6.11	101.95	109.65
1	A	97	ASP	N-CA-C	6.10	123.78	110.80
1	D	121	HIS	CA-CB-CG	5.97	119.77	113.80
1	D	134	GLY	N-CA-C	-5.97	107.00	115.30
1	D	169	ALA	N-CA-C	5.97	118.88	110.23
1	B	110	LYS	CA-C-N	-5.94	112.12	122.64
1	B	110	LYS	C-N-CA	-5.94	112.12	122.64
1	A	103	GLY	CA-C-O	-5.94	113.03	121.52
1	B	126	PRO	CB-CA-C	-5.93	103.63	111.23
1	B	72	ILE	N-CA-C	-5.93	99.81	108.11
1	D	48	VAL	N-CA-C	5.93	117.02	108.48
1	D	166	HIS	N-CA-C	5.92	119.17	110.59
1	A	189	LEU	CA-C-N	5.91	132.33	121.70
1	A	189	LEU	C-N-CA	5.91	132.33	121.70
1	D	95	ARG	NE-CZ-NH1	-5.86	115.64	121.50
1	D	102	GLY	N-CA-C	-5.76	106.26	112.08
1	D	119	GLY	O-C-N	5.75	130.69	122.81
1	D	120	HIS	CA-C-N	-5.71	112.95	120.95
1	D	120	HIS	C-N-CA	-5.71	112.95	120.95
1	B	129	GLU	CB-CG-CD	-5.67	102.97	112.60
1	D	101	ALA	N-CA-CB	5.61	118.81	110.40
1	D	133	ASP	N-CA-C	5.57	122.66	110.80
1	A	120	HIS	O-C-N	5.57	129.99	122.59
1	A	120	HIS	CA-C-O	5.55	128.45	120.51
1	A	105	PHE	CB-CA-C	5.55	119.49	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	118	MET	CA-C-N	5.54	126.20	120.60
1	D	118	MET	C-N-CA	5.54	126.20	120.60
1	D	119	GLY	CA-C-N	5.53	132.10	121.54
1	D	119	GLY	C-N-CA	5.53	132.10	121.54
1	D	99	GLU	O-C-N	5.53	129.07	122.27
1	D	96	PRO	N-CA-CB	5.48	108.63	102.60
1	D	95	ARG	CD-NE-CZ	-5.47	116.75	124.40
1	C	51	GLU	N-CA-C	5.45	122.42	110.80
1	D	99	GLU	N-CA-C	-5.43	105.53	111.82
1	B	133	ASP	CB-CA-C	-5.39	99.70	110.42
1	B	129	GLU	CG-CD-OE1	-5.37	106.04	118.40
1	C	120	HIS	CB-CA-C	5.34	121.05	110.42
1	B	51	GLU	CB-CA-C	5.24	119.59	110.94
1	B	83	LEU	CA-C-N	5.23	124.94	119.92
1	B	83	LEU	C-N-CA	5.23	124.94	119.92
1	C	101	ALA	CA-C-N	5.22	131.09	121.70
1	C	101	ALA	C-N-CA	5.22	131.09	121.70
1	D	103	GLY	O-C-N	-5.19	116.58	121.77
1	B	104	PRO	N-CA-C	5.18	119.22	111.14
1	D	101	ALA	CA-C-O	-5.17	112.01	120.80
1	A	163	PHE	N-CA-C	-5.16	100.84	109.24
1	C	94	VAL	CB-CA-C	5.13	117.17	110.96
1	D	118	MET	CB-CG-SD	-5.12	97.33	112.70
1	A	42	GLY	CA-C-N	-5.11	114.49	122.16
1	A	42	GLY	C-N-CA	-5.11	114.49	122.16
1	B	132	ALA	CA-C-N	5.08	131.25	121.54
1	B	132	ALA	C-N-CA	5.08	131.25	121.54
1	B	103	GLY	N-CA-C	-5.07	102.00	112.34
1	B	154	ASN	N-CA-C	-5.07	101.70	109.76
1	C	97	ASP	N-CA-C	5.05	121.57	110.80
1	B	129	GLU	CA-CB-CG	-5.05	104.00	114.10
1	B	112	HIS	N-CA-C	5.00	117.68	110.28

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	120	HIS	CA
1	D	101	ALA	CA

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	SER	Peptide
1	A	102	GLY	Peptide
1	A	103	GLY	Peptide
1	A	119	GLY	Mainchain
1	A	40	ALA	Peptide
1	A	42	GLY	Peptide
1	A	88	TYR	Peptide
1	B	102	GLY	Peptide
1	B	103	GLY	Peptide
1	B	119	GLY	Peptide
1	B	40	ALA	Peptide
1	B	96	PRO	Peptide
1	B	97	ASP	Mainchain,Peptide
1	C	102	GLY	Peptide
1	C	103	GLY	Mainchain,Peptide
1	C	40	ALA	Peptide
1	D	101	ALA	Mainchain,Peptide
1	D	103	GLY	Mainchain
1	D	132	ALA	Peptide
1	D	40	ALA	Peptide
1	D	64	ASP	Peptide
1	D	95	ARG	Mainchain,Peptide
1	D	96	PRO	Peptide
1	D	97	ASP	Mainchain

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	1129	0	1075	84	0
1	B	1133	0	1076	60	0
1	C	1129	0	1075	65	0
1	D	1129	0	1074	60	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	93	0	0	25	0
4	B	117	0	0	18	0
4	C	83	0	0	17	0
4	D	97	0	0	4	0
All	All	4920	0	4300	265	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 30.

All (265) 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:A:156:LEU:HD23	1:A:190:LEU:CD2	1.64	1.28
1:D:110:LYS:HE2	1:D:120:HIS:CB	1.66	1.25
1:D:156:LEU:HD21	1:D:189:LEU:HG	1.19	1.17
1:A:156:LEU:CD2	1:A:190:LEU:CD2	2.25	1.14
1:A:140:MET:HB3	4:A:894:HOH:O	1.46	1.12
1:C:156:LEU:CD1	1:C:190:LEU:HD21	1.80	1.11
1:A:156:LEU:CD2	1:A:190:LEU:HD22	1.80	1.11
1:B:89:GLU:HG2	1:B:103:GLY:HA3	1.32	1.10
1:B:120:HIS:HB3	4:B:918:HOH:O	1.49	1.10
1:C:156:LEU:HD11	1:C:190:LEU:CD2	1.81	1.10
1:B:88:TYR:HD1	1:B:103:GLY:O	1.34	1.07
1:D:110:LYS:HE2	1:D:120:HIS:HB3	1.37	1.06
1:A:156:LEU:HD23	1:A:190:LEU:HD21	1.35	1.05
1:D:110:LYS:HE2	1:D:120:HIS:HB2	1.35	1.05
1:C:50:ARG:O	1:C:51:GLU:HG3	1.58	1.02
1:A:88:TYR:HD1	1:A:103:GLY:HA3	1.28	0.99
1:C:62:GLU:HB2	4:C:681:HOH:O	1.63	0.99
1:C:167:GLU:HB3	4:C:684:HOH:O	1.63	0.96
1:C:156:LEU:HD11	1:C:190:LEU:HD21	1.01	0.96
1:A:156:LEU:CD2	1:A:190:LEU:HD21	1.93	0.94
1:C:89:GLU:CD	1:C:103:GLY:HA3	1.95	0.92
1:A:108:LEU:O	1:A:110:LYS:HE2	1.71	0.91
1:B:88:TYR:CD1	1:B:103:GLY:O	2.23	0.90
1:A:133:ASP:HB3	4:A:889:HOH:O	1.73	0.89
1:B:148:LYS:HD3	4:B:835:HOH:O	1.74	0.88
1:B:97:ASP:O	1:B:98:PHE:C	2.11	0.87
1:A:88:TYR:CD1	1:A:103:GLY:HA3	2.08	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ALA:HB1	4:B:917:HOH:O	1.74	0.87
1:A:133:ASP:OD1	1:A:135:LYS:HD2	1.75	0.86
1:C:156:LEU:CD1	1:C:190:LEU:CD2	2.48	0.86
1:B:190:LEU:HG	1:A:78:ARG:NH1	1.90	0.86
1:A:53:LYS:HG2	4:A:810:HOH:O	1.75	0.85
1:A:156:LEU:HD23	1:A:190:LEU:HD22	1.42	0.85
1:B:89:GLU:CG	1:B:103:GLY:HA3	2.06	0.85
1:A:100:SER:HB3	4:A:858:HOH:O	1.75	0.84
1:B:152:LYS:HD3	4:B:909:HOH:O	1.78	0.84
1:B:64:ASP:HA	1:B:65:ASP:CB	2.07	0.83
1:D:156:LEU:CD2	1:D:189:LEU:HG	2.06	0.82
1:D:156:LEU:HD21	1:D:189:LEU:CG	2.05	0.82
1:A:140:MET:CE	4:A:894:HOH:O	2.28	0.82
1:A:140:MET:HE3	4:A:894:HOH:O	1.78	0.81
1:B:152:LYS:CD	1:B:152:LYS:H	1.94	0.81
1:A:43:HIS:HB2	1:A:60:ILE:HG12	1.64	0.80
1:C:120:HIS:HE1	4:C:680:HOH:O	1.63	0.80
1:B:64:ASP:HA	1:B:65:ASP:CG	2.08	0.79
1:A:147:LEU:HD22	1:A:156:LEU:HD12	1.65	0.79
1:D:133:ASP:HB3	1:D:135:LYS:H	1.47	0.79
1:B:101:ALA:HB1	1:B:102:GLY:HA2	1.65	0.78
1:C:97:ASP:HA	4:C:642:HOH:O	1.83	0.78
1:D:45:VAL:CG2	1:D:58:ILE:HB	2.12	0.78
1:A:127:ASN:HD21	1:A:170:ASP:HB3	1.48	0.78
1:C:97:ASP:HB2	4:C:661:HOH:O	1.84	0.78
1:C:90:LYS:HG3	1:C:159:ASP:HB3	1.64	0.78
1:D:115:ASN:HD22	1:D:173:LEU:HD21	1.48	0.78
1:D:133:ASP:OD2	1:D:135:LYS:HD2	1.86	0.76
1:A:89:GLU:H	1:A:103:GLY:HA2	1.50	0.76
1:A:66:GLU:HG3	1:A:67:GLY:H	1.51	0.76
1:D:92:SER:HB3	1:D:101:ALA:HB3	1.66	0.76
1:C:112:HIS:HB2	1:C:121:HIS:CE1	2.21	0.75
1:A:90:LYS:HD3	4:A:834:HOH:O	1.86	0.75
1:C:53:LYS:HA	4:C:609:HOH:O	1.85	0.75
1:D:167:GLU:HG2	1:D:168:GLN:HG2	1.69	0.74
1:D:115:ASN:HD22	1:D:173:LEU:CD2	1.99	0.73
1:D:89:GLU:HG2	1:D:103:GLY:O	1.89	0.73
1:C:95:ARG:HD3	4:C:655:HOH:O	1.89	0.72
1:D:179:ASN:CG	4:D:797:HOH:O	2.32	0.72
1:A:46:GLN:HG2	4:A:809:HOH:O	1.87	0.72
1:D:94:VAL:HB	1:D:100:SER:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:VAL:HG23	1:D:45:VAL:O	1.90	0.71
1:C:118:MET:HG3	4:C:668:HOH:O	1.89	0.71
1:A:66:GLU:HG3	1:A:67:GLY:N	2.04	0.71
1:A:40:ALA:HB1	4:C:656:HOH:O	1.89	0.70
1:B:97:ASP:O	1:B:99:GLU:N	2.24	0.70
1:C:147:LEU:HD12	4:C:681:HOH:O	1.91	0.70
1:B:65:ASP:HB2	4:B:913:HOH:O	1.90	0.70
1:B:100:SER:CB	4:B:887:HOH:O	2.38	0.70
1:A:156:LEU:HD21	1:A:190:LEU:HD22	1.70	0.68
1:D:110:LYS:CE	1:D:120:HIS:HB3	2.21	0.68
1:D:45:VAL:HG21	1:D:58:ILE:HB	1.77	0.66
1:B:101:ALA:HB1	1:B:102:GLY:CA	2.26	0.66
1:A:63:SER:C	1:A:65:ASP:HA	2.22	0.65
1:B:111:GLU:HG3	1:B:116:ASN:ND2	2.12	0.65
1:C:96:PRO:HG2	1:C:97:ASP:OD1	1.97	0.65
1:C:149:LYS:HA	1:C:154:ASN:HD22	1.60	0.65
1:D:115:ASN:HB2	1:D:173:LEU:HD22	1.79	0.64
1:B:64:ASP:HA	1:B:65:ASP:HB3	1.78	0.64
1:D:179:ASN:HB3	4:D:797:HOH:O	1.96	0.64
1:C:120:HIS:CE1	4:C:680:HOH:O	2.42	0.64
1:B:127:ASN:HD21	1:B:170:ASP:HB3	1.63	0.63
1:B:177:SER:CB	4:B:830:HOH:O	2.47	0.63
1:A:99:GLU:HB2	4:A:865:HOH:O	1.99	0.63
1:A:99:GLU:O	1:A:101:ALA:HA	1.99	0.63
1:C:112:HIS:H	1:C:175:ASN:HD21	1.46	0.62
1:A:43:HIS:HB2	1:A:60:ILE:CG1	2.29	0.62
1:C:127:ASN:HD21	1:C:170:ASP:HB3	1.64	0.62
1:A:99:GLU:CB	4:A:865:HOH:O	2.48	0.62
1:A:78:ARG:NH2	4:A:864:HOH:O	2.33	0.61
1:B:152:LYS:HD2	1:B:152:LYS:N	2.15	0.60
1:C:86:HIS:HB2	1:C:88:TYR:CE2	2.35	0.60
1:D:115:ASN:HB2	1:D:173:LEU:CD2	2.32	0.60
1:D:127:ASN:HD21	1:D:170:ASP:HB3	1.65	0.60
1:A:127:ASN:HD21	1:A:170:ASP:CB	2.13	0.60
1:D:110:LYS:HG3	1:D:120:HIS:HB3	1.83	0.60
1:A:125:LEU:HB3	1:A:126:PRO:CD	2.33	0.59
1:B:100:SER:HB3	4:B:887:HOH:O	2.00	0.59
1:B:66:GLU:HB3	4:B:913:HOH:O	2.03	0.59
1:B:129:GLU:CG	4:B:873:HOH:O	2.50	0.58
1:A:110:LYS:CD	4:A:861:HOH:O	2.51	0.58
1:C:133:ASP:HB3	1:C:135:LYS:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:HIS:HB2	1:A:124:ASP:CG	2.29	0.58
1:B:152:LYS:HG2	4:B:894:HOH:O	2.03	0.58
1:C:50:ARG:O	1:C:51:GLU:CG	2.44	0.58
1:D:168:GLN:HB3	4:D:770:HOH:O	2.02	0.58
1:C:53:LYS:HG2	4:C:609:HOH:O	2.04	0.58
1:D:116:ASN:HB3	1:D:119:GLY:HA3	1.86	0.58
1:A:156:LEU:HD22	1:A:190:LEU:HD21	1.84	0.57
1:A:147:LEU:HD22	1:A:156:LEU:CD1	2.32	0.57
1:D:106:ASN:ND2	1:D:109:ASN:HA	2.19	0.57
1:C:111:GLU:O	1:C:120:HIS:N	2.34	0.57
1:B:127:ASN:HD21	1:B:170:ASP:H	1.53	0.56
1:C:62:GLU:CA	4:C:681:HOH:O	2.53	0.56
1:D:179:ASN:CB	4:D:797:HOH:O	2.52	0.56
1:A:92:SER:OG	1:A:100:SER:O	2.23	0.56
1:A:90:LYS:CE	4:A:873:HOH:O	2.53	0.56
1:A:90:LYS:HE3	4:A:873:HOH:O	2.06	0.56
1:D:45:VAL:CG2	1:D:45:VAL:O	2.54	0.56
1:D:110:LYS:CE	1:D:120:HIS:HB2	2.23	0.56
1:B:151:SER:HA	4:B:909:HOH:O	2.05	0.56
1:C:49:ASN:O	1:C:51:GLU:N	2.34	0.56
1:D:172:TYR:C	1:D:173:LEU:HD23	2.31	0.56
1:A:125:LEU:HB3	1:A:126:PRO:HD3	1.87	0.55
1:B:190:LEU:HG	1:A:78:ARG:HH12	1.67	0.55
1:D:106:ASN:HD21	1:D:109:ASN:HA	1.72	0.55
1:B:99:GLU:O	1:B:101:ALA:HA	2.07	0.54
1:A:110:LYS:HD3	4:A:861:HOH:O	2.07	0.54
1:C:65:ASP:CB	1:C:66:GLU:HA	2.38	0.54
1:B:97:ASP:C	4:B:892:HOH:O	2.50	0.54
1:A:140:MET:CG	4:A:894:HOH:O	2.54	0.53
1:B:177:SER:HB2	4:B:830:HOH:O	2.08	0.53
1:A:50:ARG:HD3	4:A:820:HOH:O	2.08	0.53
1:C:127:ASN:HD21	1:C:170:ASP:CB	2.21	0.53
1:C:99:GLU:O	1:C:101:ALA:HA	2.08	0.53
1:D:50:ARG:HG2	1:D:96:PRO:O	2.09	0.53
1:A:66:GLU:CG	1:A:67:GLY:N	2.72	0.52
1:A:98:PHE:C	1:A:100:SER:H	2.16	0.52
1:A:47:LEU:HD21	1:A:58:ILE:HD12	1.91	0.52
1:D:127:ASN:HD21	1:D:170:ASP:H	1.58	0.52
1:C:62:GLU:HA	4:C:681:HOH:O	2.07	0.52
1:D:121:HIS:HB2	1:D:124:ASP:CG	2.35	0.52
1:B:66:GLU:HG2	4:B:891:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:HIS:HB2	1:A:121:HIS:CE1	2.46	0.51
1:B:63:SER:O	1:B:65:ASP:HB3	2.11	0.51
1:C:64:ASP:HA	1:C:65:ASP:OD2	2.11	0.51
1:A:158:GLU:HB2	4:A:887:HOH:O	2.10	0.51
1:C:127:ASN:HD21	1:C:170:ASP:H	1.57	0.51
1:D:168:GLN:HG3	1:D:180:SER:O	2.10	0.51
1:B:89:GLU:CD	1:B:103:GLY:CA	2.83	0.51
1:A:97:ASP:O	1:A:99:GLU:N	2.44	0.51
1:A:63:SER:O	1:A:65:ASP:HA	2.10	0.51
1:B:152:LYS:HD3	1:B:152:LYS:H	1.73	0.51
1:C:40:ALA:N	1:C:61:LYS:HG3	2.26	0.50
1:C:62:GLU:CB	4:C:681:HOH:O	2.34	0.50
1:A:100:SER:CB	4:A:858:HOH:O	2.45	0.50
1:C:92:SER:OG	1:C:94:VAL:HG23	2.12	0.50
1:C:57:PHE:CE2	1:C:59:GLU:HG3	2.47	0.50
1:B:127:ASN:HD21	1:B:170:ASP:CB	2.25	0.50
1:C:156:LEU:CD1	1:C:190:LEU:HD23	2.39	0.50
1:D:116:ASN:O	1:D:119:GLY:N	2.40	0.49
1:A:49:ASN:C	1:A:49:ASN:OD1	2.54	0.49
1:C:108:LEU:N	1:C:108:LEU:HD12	2.27	0.49
1:C:159:ASP:HB2	4:C:677:HOH:O	2.12	0.49
1:D:77:LEU:O	1:D:79:PRO:HD3	2.13	0.49
1:A:126:PRO:HD2	1:A:140:MET:SD	2.53	0.49
1:B:89:GLU:CD	1:B:103:GLY:HA3	2.37	0.49
1:C:89:GLU:CG	1:C:103:GLY:HA3	2.43	0.49
1:D:89:GLU:HG2	1:D:103:GLY:H	1.78	0.49
1:B:158:GLU:HB2	4:B:866:HOH:O	2.12	0.48
1:C:49:ASN:OD1	1:C:51:GLU:HB2	2.14	0.48
1:C:63:SER:OG	1:C:64:ASP:N	2.46	0.48
1:C:127:ASN:ND2	1:C:170:ASP:H	2.11	0.48
1:A:65:ASP:HB3	1:A:66:GLU:HA	1.95	0.48
1:D:115:ASN:O	1:D:117:PRO:HD3	2.14	0.48
1:C:65:ASP:HB3	1:C:66:GLU:HA	1.95	0.48
1:B:118:MET:HE2	1:B:118:MET:HA	1.94	0.48
1:C:49:ASN:C	1:C:51:GLU:N	2.72	0.48
1:D:164:ILE:HG21	1:D:183:ARG:HB3	1.95	0.48
1:A:125:LEU:CB	1:A:126:PRO:CD	2.92	0.47
1:A:127:ASN:ND2	1:A:170:ASP:HB3	2.25	0.47
1:D:45:VAL:HG22	1:D:58:ILE:O	2.13	0.47
1:C:165:ILE:HB	1:C:185:VAL:HB	1.95	0.47
1:A:110:LYS:HD2	4:A:861:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:LEU:HG	1:C:56:GLY:C	2.40	0.47
1:B:111:GLU:HG3	1:B:116:ASN:HD21	1.80	0.47
1:B:65:ASP:HB2	1:B:66:GLU:CB	2.45	0.47
1:A:156:LEU:HD22	1:A:190:LEU:CD2	2.33	0.46
1:B:95:ARG:HG3	4:A:830:HOH:O	2.15	0.46
1:A:90:LYS:NZ	4:A:873:HOH:O	2.48	0.46
1:A:147:LEU:CD2	1:A:156:LEU:HD12	2.41	0.46
1:A:140:MET:CB	4:A:894:HOH:O	2.24	0.46
1:D:43:HIS:HB2	1:D:60:ILE:HG12	1.98	0.45
1:A:102:GLY:O	1:A:183:ARG:NH1	2.42	0.45
1:C:89:GLU:OE2	1:C:103:GLY:HA3	2.13	0.45
1:D:110:LYS:CG	1:D:120:HIS:HB3	2.44	0.45
1:B:119:GLY:O	1:B:120:HIS:HB2	2.15	0.45
1:C:157:ASP:O	1:C:158:GLU:C	2.58	0.45
1:B:120:HIS:CG	4:B:918:HOH:O	2.65	0.45
1:C:48:VAL:O	1:C:185:VAL:HA	2.17	0.45
1:D:119:GLY:O	1:D:120:HIS:HB2	2.17	0.45
1:C:63:SER:HB3	1:C:67:GLY:O	2.18	0.44
1:C:116:ASN:HA	1:C:173:LEU:HD23	1.99	0.44
1:A:97:ASP:O	1:A:98:PHE:C	2.61	0.44
1:C:49:ASN:C	1:C:51:GLU:H	2.25	0.44
1:A:88:TYR:HB3	1:A:103:GLY:HA3	2.00	0.44
1:D:53:LYS:HD2	1:D:55:VAL:HG12	1.99	0.44
1:A:133:ASP:CB	4:A:889:HOH:O	2.49	0.44
1:D:85:PHE:CE2	1:D:140:MET:SD	3.11	0.44
1:C:128:LEU:HD22	1:C:136:VAL:HG21	1.99	0.44
1:C:64:ASP:HA	1:C:65:ASP:CG	2.44	0.43
1:C:98:PHE:C	1:C:100:SER:N	2.72	0.43
1:D:45:VAL:HG22	1:D:58:ILE:HB	1.98	0.43
1:D:72:ILE:HD11	1:D:165:ILE:HD11	2.00	0.43
1:D:99:GLU:O	1:D:101:ALA:C	2.61	0.43
1:B:128:LEU:HD22	1:B:136:VAL:HG21	1.99	0.43
1:B:85:PHE:HE2	1:B:140:MET:SD	2.41	0.43
1:A:128:LEU:HD22	1:A:136:VAL:HG21	2.01	0.43
1:B:47:LEU:HD23	1:B:47:LEU:HA	1.75	0.43
1:A:55:VAL:HA	1:A:75:ASN:HD21	1.84	0.43
1:A:89:GLU:CD	1:A:103:GLY:O	2.62	0.43
1:D:90:LYS:HB2	1:D:101:ALA:HB1	2.00	0.43
1:B:120:HIS:CB	4:B:918:HOH:O	2.31	0.43
1:A:127:ASN:HD21	1:A:170:ASP:H	1.67	0.43
1:D:75:ASN:C	1:D:75:ASN:HD22	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:GLU:OE2	1:D:118:MET:HE2	2.19	0.43
1:D:110:LYS:HG3	1:D:120:HIS:O	2.19	0.42
1:B:64:ASP:CA	1:B:65:ASP:CG	2.88	0.42
1:B:99:GLU:C	1:B:101:ALA:HA	2.44	0.42
1:A:125:LEU:CD2	1:A:142:ALA:HB2	2.49	0.42
1:B:64:ASP:O	1:D:64:ASP:OD2	2.38	0.42
1:C:100:SER:HA	1:C:101:ALA:HB2	2.01	0.42
1:A:78:ARG:HE	1:A:81:ALA:HB2	1.84	0.42
1:A:121:HIS:HB2	1:A:124:ASP:OD2	2.19	0.42
1:C:51:GLU:C	1:C:53:LYS:H	2.27	0.42
1:C:53:LYS:CA	4:C:609:HOH:O	2.56	0.42
1:D:127:ASN:HD21	1:D:170:ASP:CB	2.30	0.42
1:B:65:ASP:HB2	1:B:66:GLU:HB3	2.01	0.42
1:A:74:ALA:HB3	1:A:136:VAL:CG1	2.50	0.42
1:B:65:ASP:CB	1:B:66:GLU:HA	2.49	0.42
1:C:58:ILE:HA	1:C:71:HIS:O	2.20	0.42
1:B:64:ASP:CA	1:B:65:ASP:CB	2.90	0.41
1:B:127:ASN:ND2	1:B:170:ASP:H	2.18	0.41
1:A:78:ARG:HA	1:A:79:PRO:HD3	1.94	0.41
1:B:110:LYS:HE3	1:B:110:LYS:HB3	1.87	0.41
1:B:190:LEU:CG	1:A:78:ARG:NH1	2.74	0.41
1:D:95:ARG:HH11	1:D:95:ARG:HD2	1.54	0.41
1:A:88:TYR:OH	1:A:166:HIS:NE2	2.38	0.41
1:A:100:SER:C	4:A:804:HOH:O	2.62	0.41
1:C:122:ALA:HB1	1:C:144:ASP:O	2.21	0.41
1:C:149:LYS:HA	1:C:154:ASN:ND2	2.33	0.41
1:D:50:ARG:HE	1:D:50:ARG:HB2	1.59	0.41
1:D:58:ILE:HD11	1:D:72:ILE:HD12	2.03	0.41
1:A:68:LEU:CD1	1:A:155:ILE:HD11	2.51	0.41
1:B:152:LYS:H	1:B:152:LYS:HD2	1.68	0.40
1:A:88:TYR:HB3	1:A:103:GLY:CA	2.52	0.40
1:A:164:ILE:HD13	1:A:183:ARG:HD3	2.04	0.40
1:D:97:ASP:C	1:D:99:GLU:N	2.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	149/175 (85%)	132 (89%)	15 (10%)	2 (1%)	9	3
1	B	150/175 (86%)	134 (89%)	10 (7%)	6 (4%)	2	0
1	C	149/175 (85%)	125 (84%)	15 (10%)	9 (6%)	1	0
1	D	149/175 (85%)	136 (91%)	9 (6%)	4 (3%)	4	0
All	All	597/700 (85%)	527 (88%)	49 (8%)	21 (4%)	3	0

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	97	ASP
1	B	98	PHE
1	B	120	HIS
1	B	133	ASP
1	A	120	HIS
1	D	120	HIS
1	D	133	ASP
1	C	51	GLU
1	C	97	ASP
1	C	133	ASP
1	C	158	GLU
1	C	53	LYS
1	C	120	HIS
1	D	98	PHE
1	C	103	GLY
1	D	42	GLY
1	A	42	GLY
1	C	42	GLY
1	C	96	PRO
1	B	103	GLY
1	B	96	PRO

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	120/143 (84%)	105 (88%)	15 (12%)	4	1
1	B	120/143 (84%)	100 (83%)	20 (17%)	2	0
1	C	120/143 (84%)	103 (86%)	17 (14%)	3	1
1	D	120/143 (84%)	101 (84%)	19 (16%)	2	0
All	All	480/572 (84%)	409 (85%)	71 (15%)	3	0

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	45	VAL
1	B	46	GLN
1	B	50	ARG
1	B	51	GLU
1	B	61	LYS
1	B	65	ASP
1	B	66	GLU
1	B	90	LYS
1	B	100	SER
1	B	108	LEU
1	B	126	PRO
1	B	129	GLU
1	B	133	ASP
1	B	148	LYS
1	B	149	LYS
1	B	152	LYS
1	B	156	LEU
1	B	159	ASP
1	B	177	SER
1	B	190	LEU
1	A	45	VAL
1	A	50	ARG
1	A	53	LYS
1	A	64	ASP

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Mol	Chain	Res	Type
1	A	75	ASN
1	A	92	SER
1	A	100	SER
1	A	108	LEU
1	A	110	LYS
1	A	118	MET
1	A	120	HIS
1	A	125	LEU
1	A	129	GLU
1	A	152	LYS
1	A	190	LEU
1	C	45	VAL
1	C	46	GLN
1	C	47	LEU
1	C	53	LYS
1	C	62	GLU
1	C	65	ASP
1	C	72	ILE
1	C	76	SER
1	C	95	ARG
1	C	120	HIS
1	C	133	ASP
1	C	136	VAL
1	C	148	LYS
1	C	149	LYS
1	C	168	GLN
1	C	173	LEU
1	C	190	LEU
1	D	53	LYS
1	D	64	ASP
1	D	65	ASP
1	D	75	ASN
1	D	82	SER
1	D	92	SER
1	D	95	ARG
1	D	97	ASP
1	D	108	LEU
1	D	110	LYS
1	D	120	HIS
1	D	140	MET
1	D	149	LYS
1	D	151	SER

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Mol	Chain	Res	Type
1	D	152	LYS
1	D	167	GLU
1	D	168	GLN
1	D	173	LEU
1	D	190	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	115	ASN
1	B	120	HIS
1	B	127	ASN
1	A	75	ASN
1	A	127	ASN
1	C	75	ASN
1	C	127	ASN
1	C	175	ASN
1	D	75	ASN
1	D	109	ASN
1	D	115	ASN
1	D	127	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 10 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	2
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	102:GLY	C	103:GLY	N	1.17
1	D	65:ASP	C	66:GLU	N	1.14
1	B	96:PRO	C	97:ASP	N	1.12
1	B	97:ASP	C	98:PHE	N	1.12

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, 95th 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	151/175 (86%)	1.17	26 (17%) 4 3	17, 39, 51, 61	0
1	B	152/175 (86%)	0.74	14 (9%) 14 12	16, 33, 50, 63	0
1	C	151/175 (86%)	1.38	29 (19%) 3 2	17, 40, 58, 70	0
1	D	151/175 (86%)	1.22	23 (15%) 5 4	17, 38, 51, 57	0
All	All	605/700 (86%)	1.13	92 (15%) 5 4	16, 38, 54, 70	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	103	GLY	6.0
1	B	97	ASP	5.9
1	D	101	ALA	5.9
1	D	120	HIS	5.9
1	A	120	HIS	5.4
1	D	65	ASP	5.3
1	D	97	ASP	5.1
1	D	100	SER	5.0
1	D	102	GLY	4.9
1	C	96	PRO	4.7
1	C	99	GLU	4.6
1	B	101	ALA	4.5
1	C	40	ALA	4.4
1	D	119	GLY	4.2
1	C	100	SER	4.2
1	C	101	ALA	4.2
1	B	102	GLY	4.2
1	A	102	GLY	4.0
1	C	102	GLY	3.9
1	D	103	GLY	3.9
1	C	41	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	190	LEU	3.6
1	A	119	GLY	3.5
1	C	42	GLY	3.5
1	B	103	GLY	3.3
1	D	96	PRO	3.3
1	A	101	ALA	3.2
1	D	109	ASN	3.2
1	A	100	SER	3.2
1	D	42	GLY	3.2
1	C	54	ALA	3.2
1	D	98	PHE	3.2
1	C	168	GLN	3.2
1	A	40	ALA	3.1
1	B	96	PRO	3.1
1	C	190	LEU	3.0
1	A	96	PRO	3.0
1	C	65	ASP	3.0
1	C	103	GLY	3.0
1	B	100	SER	3.0
1	D	116	ASN	2.8
1	C	55	VAL	2.8
1	B	40	ALA	2.7
1	C	45	VAL	2.7
1	A	118	MET	2.6
1	D	133	ASP	2.6
1	A	43	HIS	2.6
1	C	64	ASP	2.6
1	D	156	LEU	2.5
1	A	52	GLY	2.5
1	C	63	SER	2.5
1	C	151	SER	2.5
1	B	140	MET	2.5
1	B	120	HIS	2.4
1	A	64	ASP	2.4
1	D	169	ALA	2.4
1	D	40	ALA	2.4
1	A	104	PRO	2.4
1	D	190	LEU	2.3
1	D	174	THR	2.3
1	C	47	LEU	2.3
1	A	44	HIS	2.3
1	A	42	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	173	LEU	2.3
1	C	56	GLY	2.3
1	C	184	ILE	2.3
1	B	46	GLN	2.2
1	B	157	ASP	2.2
1	A	177	SER	2.2
1	C	75	ASN	2.2
1	B	109	ASN	2.2
1	A	75	ASN	2.2
1	D	118	MET	2.2
1	C	94	VAL	2.2
1	C	157	ASP	2.2
1	D	179	ASN	2.1
1	A	189	LEU	2.1
1	C	98	PHE	2.1
1	A	133	ASP	2.1
1	A	94	VAL	2.1
1	D	66	GLU	2.0
1	B	119	GLY	2.0
1	C	43	HIS	2.0
1	C	44	HIS	2.0
1	A	126	PRO	2.0
1	C	93	CYS	2.0
1	B	64	ASP	2.0
1	A	159	ASP	2.0
1	C	50	ARG	2.0
1	A	91	GLY	2.0
1	A	79	PRO	2.0
1	A	136	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZN	A	802	1/1	0.92	0.10	32,32,32,32	0
2	ZN	A	501	1/1	0.95	0.07	36,36,36,36	0
3	CL	A	502	1/1	0.96	0.09	34,34,34,34	0
3	CL	B	402	1/1	0.97	0.06	28,28,28,28	0
2	ZN	B	801	1/1	0.97	0.10	27,27,27,27	0
2	ZN	B	401	1/1	0.98	0.06	33,33,33,33	0
2	ZN	C	601	1/1	0.98	0.08	33,33,33,33	0
3	CL	D	702	1/1	0.98	0.06	38,38,38,38	0
3	CL	C	602	1/1	0.99	0.05	30,30,30,30	0
2	ZN	D	701	1/1	0.99	0.05	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.