



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:53 PM UTC

PDB ID : 1XTL / pdb_00001xtl
Title : Crystal structure of P104H mutant of SOD-like protein from *Bacillus subtilis*.
Authors : Calderone, V.; Mangani, S.; Banci, L.; Benvenuti, M.; Bertini, I.; Viezzoli, M.S.; Fantoni, A.
Deposited on : 2004-10-22
Resolution : 2.00 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

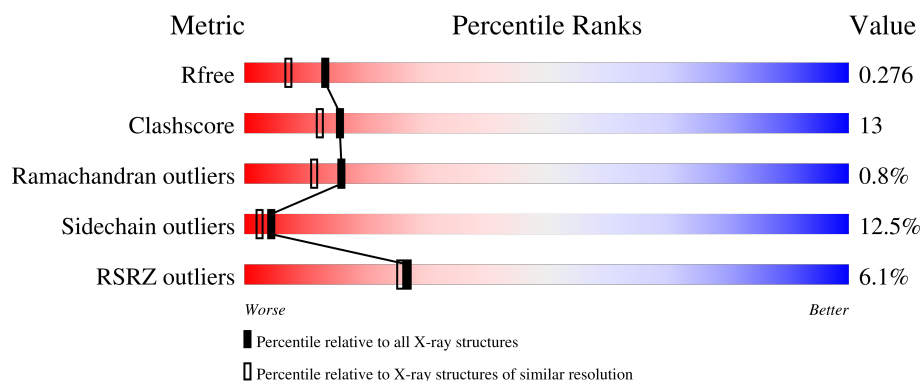
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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

There are 4 unique types of molecules in this entry. The entry contains 4865 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 Hypothetical superoxide dismutase-like protein yojM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	152	Total	C	N	O	S	1	0	0
			1136	705	203	224	4			
1	A	152	Total	C	N	O	S	2	0	0
			1136	705	203	224	4			
1	C	152	Total	C	N	O	S	1	0	0
			1136	705	203	224	4			
1	D	152	Total	C	N	O	S	1	0	0
			1136	705	203	224	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	104	HIS	PRO	engineered mutation	UNP O31851
A	104	HIS	PRO	engineered mutation	UNP O31851
C	104	HIS	PRO	engineered mutation	UNP O31851
D	104	HIS	PRO	engineered mutation	UNP O31851

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total 3	Zn 3	0	0
3	A	3	Total 3	Zn 3	0	0
3	C	2	Total 2	Zn 2	0	0
3	D	2	Total 2	Zn 2	0	0

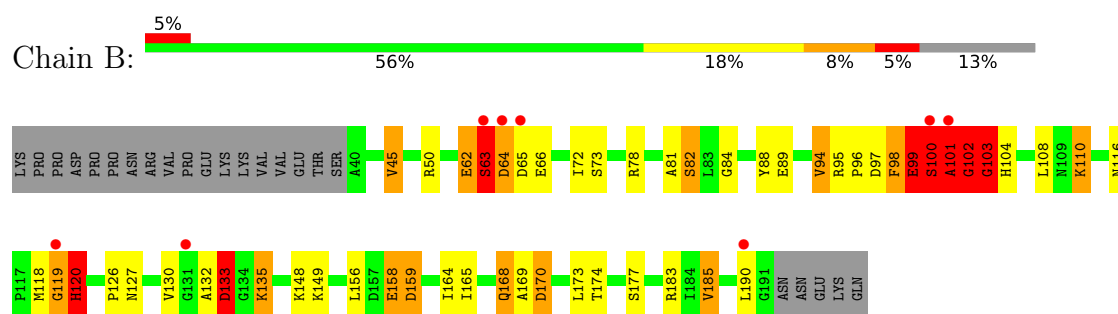
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	84	Total 84	O 84	1	0
4	A	86	Total 86	O 86	0	0
4	C	70	Total 70	O 70	1	0
4	D	67	Total 67	O 67	1	0

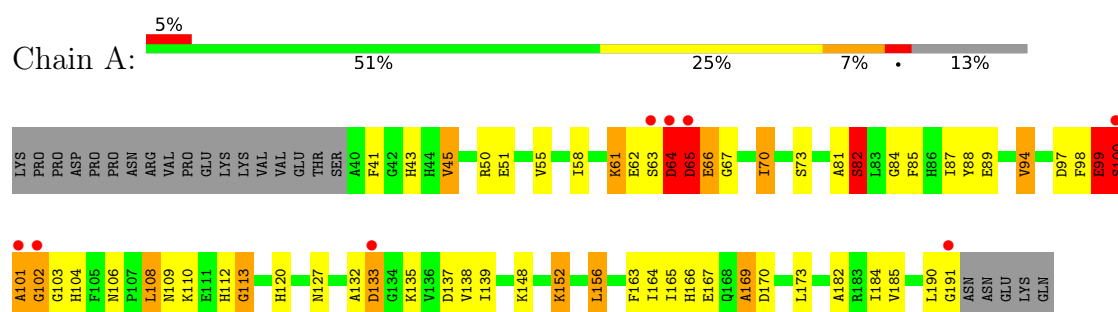
3 Residue-property plots [i](#)

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.

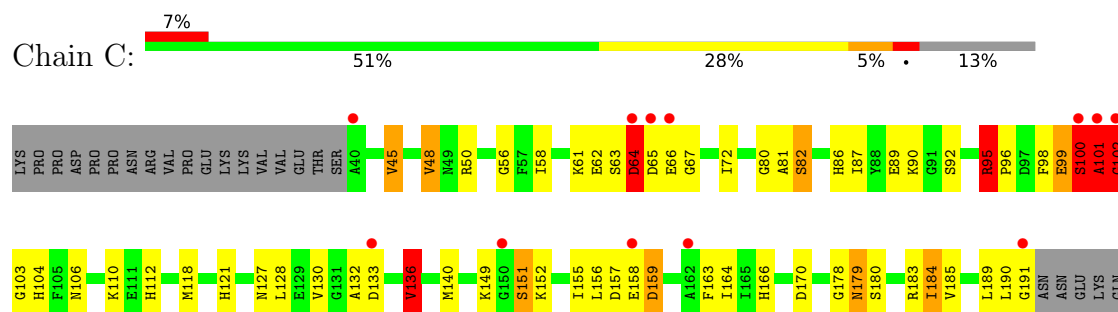
- Molecule 1: Hypothetical superoxide dismutase-like protein yojM



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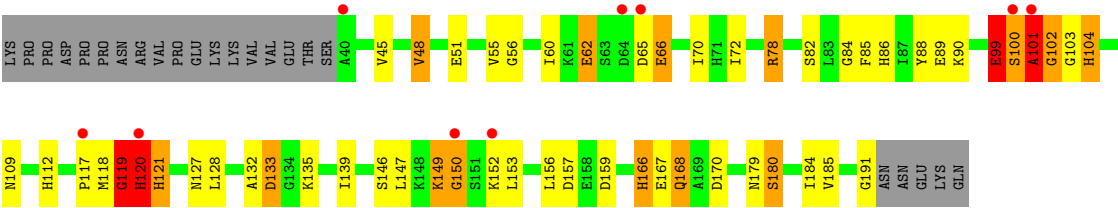


- Molecule 1: Hypothetical superoxide dismutase-like protein yojM



- Molecule 1: Hypothetical 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	52.15Å 56.59Å 59.12Å 78.24° 89.91° 85.47°	Depositor
Resolution (Å)	38.92 – 2.00 38.92 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.92-2.00) 89.9 (38.92-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.232 , 0.299 (Not available) , 0.276	Depositor DCC
R_{free} test set	6723 reflections (8.31%)	wwPDB-VP
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.792	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4865	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.06% 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: CU, 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	2.01	25/1160 (2.2%)	1.84	34/1566 (2.2%)
1	B	1.89	21/1160 (1.8%)	1.99	44/1566 (2.8%)
1	C	1.90	20/1160 (1.7%)	1.78	26/1566 (1.7%)
1	D	2.04	24/1160 (2.1%)	1.97	28/1566 (1.8%)
All	All	1.96	90/4640 (1.9%)	1.90	132/6264 (2.1%)

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	4
1	B	0	4
1	C	0	4
1	D	0	5
All	All	0	17

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	150	GLY	C-O	27.80	1.54	1.24
1	A	65	ASP	C-N	23.04	1.65	1.33
1	C	95	ARG	NE-CZ	19.35	1.54	1.33
1	C	95	ARG	CD-NE	15.61	1.68	1.46
1	A	65	ASP	C-O	-13.91	1.05	1.23
1	D	72	ILE	CA-CB	11.69	1.68	1.54
1	B	45	VAL	CA-CB	10.55	1.67	1.54
1	C	102	GLY	N-CA	10.05	1.61	1.45
1	B	50	ARG	CZ-NH2	-9.53	1.21	1.33
1	A	45	VAL	CA-CB	9.44	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	ILE	CA-CB	9.10	1.66	1.54
1	B	185	VAL	CA-CB	9.08	1.67	1.54
1	B	94	VAL	CA-CB	9.00	1.64	1.54
1	D	102	GLY	N-CA	8.53	1.59	1.45
1	B	130	VAL	CA-CB	8.36	1.64	1.54
1	D	101	ALA	CA-C	8.20	1.70	1.52
1	D	121	HIS	C-O	-8.04	1.14	1.23
1	C	101	ALA	CA-C	8.00	1.69	1.52
1	C	72	ILE	CA-CB	7.83	1.63	1.54
1	C	155	ILE	CA-CB	7.75	1.64	1.54
1	A	185	VAL	CA-CB	7.71	1.65	1.54
1	B	101	ALA	CA-C	7.65	1.69	1.52
1	A	165	ILE	CA-CB	7.35	1.63	1.54
1	D	104	HIS	CA-CB	7.35	1.65	1.53
1	B	119	GLY	N-CA	-7.30	1.37	1.44
1	D	82	SER	CA-C	7.15	1.61	1.52
1	C	184	ILE	N-CA	6.99	1.53	1.46
1	B	126	PRO	C-O	6.92	1.31	1.23
1	B	64	ASP	C-N	6.80	1.42	1.33
1	B	82	SER	N-CA	6.71	1.54	1.46
1	A	138	VAL	CA-C	-6.64	1.45	1.52
1	D	100	SER	N-CA	-6.58	1.37	1.46
1	A	182	ALA	CA-CB	6.56	1.64	1.53
1	C	45	VAL	CA-CB	6.55	1.62	1.54
1	A	87	ILE	CA-CB	6.40	1.61	1.54
1	C	102	GLY	CA-C	6.39	1.63	1.52
1	D	70	ILE	CA-CB	6.39	1.62	1.53
1	C	101	ALA	C-N	6.38	1.42	1.33
1	D	101	ALA	C-N	6.37	1.42	1.33
1	C	164	ILE	CA-CB	6.35	1.63	1.54
1	C	163	PHE	N-CA	6.34	1.53	1.46
1	C	81	ALA	N-CA	6.31	1.53	1.45
1	B	102	GLY	N-CA	6.29	1.55	1.45
1	A	102	GLY	N-CA	6.21	1.55	1.45
1	D	60	ILE	CA-CB	6.06	1.63	1.54
1	D	55	VAL	CA-CB	6.04	1.62	1.54
1	C	58	ILE	C-O	5.99	1.29	1.24
1	A	82	SER	N-CA	5.98	1.53	1.46
1	A	70	ILE	CA-CB	5.97	1.61	1.53
1	B	170	ASP	CA-C	5.92	1.60	1.52
1	B	104	HIS	CA-CB	5.89	1.62	1.53
1	A	101	ALA	CA-C	5.83	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	GLU	CD-OE1	-5.83	1.14	1.25
1	A	164	ILE	N-CA	5.75	1.52	1.46
1	D	166	HIS	CA-C	5.72	1.60	1.52
1	C	185	VAL	N-CA	5.66	1.52	1.46
1	D	139	ILE	CA-CB	5.66	1.61	1.54
1	D	119	GLY	C-N	-5.66	1.25	1.33
1	B	169	ALA	CA-CB	5.65	1.62	1.53
1	A	112	HIS	N-CA	-5.65	1.38	1.46
1	D	159	ASP	CB-CG	-5.63	1.38	1.52
1	B	120	HIS	CD2-NE2	-5.62	1.31	1.37
1	B	120	HIS	N-CA	-5.60	1.39	1.46
1	C	48	VAL	CA-CB	5.58	1.64	1.54
1	B	174	THR	CA-CB	5.56	1.62	1.53
1	D	133	ASP	CG-OD2	5.56	1.35	1.25
1	C	82	SER	CA-C	5.47	1.59	1.52
1	A	139	ILE	CA-C	5.46	1.59	1.52
1	A	85	PHE	N-CA	-5.46	1.40	1.46
1	D	101	ALA	CA-CB	-5.43	1.34	1.52
1	D	119	GLY	N-CA	-5.42	1.38	1.45
1	A	88	TYR	CA-C	-5.41	1.45	1.53
1	D	48	VAL	N-CA	5.41	1.52	1.46
1	C	189	LEU	N-CA	-5.38	1.39	1.46
1	A	94	VAL	CA-CB	5.37	1.60	1.54
1	B	119	GLY	C-N	-5.37	1.26	1.33
1	A	55	VAL	CA-C	5.36	1.59	1.52
1	D	133	ASP	CA-CB	5.29	1.62	1.53
1	C	86	HIS	C-O	5.18	1.30	1.23
1	B	73	SER	CA-C	5.18	1.59	1.53
1	A	113	GLY	C-O	5.18	1.30	1.23
1	A	138	VAL	CA-CB	5.12	1.63	1.55
1	A	99	GLU	C-O	-5.12	1.17	1.24
1	B	177	SER	N-CA	5.11	1.52	1.46
1	B	100	SER	CB-OG	5.10	1.52	1.42
1	A	81	ALA	CA-C	5.10	1.59	1.52
1	D	184	ILE	CA-C	5.07	1.60	1.52
1	D	185	VAL	CA-CB	5.06	1.62	1.54
1	D	104	HIS	CA-C	5.03	1.59	1.52
1	C	159	ASP	CB-CG	-5.00	1.39	1.52

All (132) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	150	GLY	O-C-N	-20.71	93.89	122.27
1	C	95	ARG	NE-CZ-NH1	-19.44	102.06	121.50
1	C	95	ARG	NE-CZ-NH2	18.43	135.78	119.20
1	D	119	GLY	CA-C-N	17.71	155.37	121.54
1	D	119	GLY	C-N-CA	17.71	155.37	121.54
1	B	50	ARG	NE-CZ-NH2	17.57	135.02	119.20
1	B	119	GLY	CA-C-N	17.03	154.07	121.54
1	B	119	GLY	C-N-CA	17.03	154.07	121.54
1	C	95	ARG	CD-NE-CZ	16.48	147.47	124.40
1	B	50	ARG	NH1-CZ-NH2	-14.81	100.05	119.30
1	A	65	ASP	CA-C-O	-13.05	106.90	121.51
1	A	64	ASP	O-C-N	-12.57	108.46	123.29
1	D	78	ARG	NE-CZ-NH2	12.11	130.10	119.20
1	C	102	GLY	CA-C-N	11.65	142.66	121.70
1	C	102	GLY	C-N-CA	11.65	142.66	121.70
1	D	119	GLY	CA-C-O	-11.62	111.12	121.58
1	A	99	GLU	CA-C-N	11.08	141.65	121.70
1	A	99	GLU	C-N-CA	11.08	141.65	121.70
1	D	102	GLY	CA-C-N	10.72	141.01	121.70
1	D	102	GLY	C-N-CA	10.72	141.01	121.70
1	A	64	ASP	CA-C-N	-10.61	105.39	122.36
1	A	64	ASP	C-N-CA	-10.61	105.39	122.36
1	B	120	HIS	CA-CB-CG	10.06	123.86	113.80
1	A	100	SER	CA-C-N	9.92	139.55	121.70
1	A	100	SER	C-N-CA	9.92	139.55	121.70
1	D	56	GLY	N-CA-C	9.38	121.03	111.56
1	D	78	ARG	NH1-CZ-NH2	-9.28	107.23	119.30
1	B	102	GLY	CA-C-N	9.28	138.40	121.70
1	B	102	GLY	C-N-CA	9.28	138.40	121.70
1	D	150	GLY	CA-C-O	-9.05	103.50	119.34
1	C	136	VAL	N-CA-C	-8.99	95.04	108.17
1	D	119	GLY	N-CA-C	8.98	123.76	111.54
1	D	100	SER	CA-C-N	8.87	137.67	121.70
1	D	100	SER	C-N-CA	8.87	137.67	121.70
1	D	101	ALA	N-CA-CB	-8.77	97.25	110.40
1	C	132	ALA	CA-C-N	8.74	132.71	120.29
1	C	132	ALA	C-N-CA	8.74	132.71	120.29
1	A	102	GLY	CA-C-N	8.53	137.06	121.70
1	A	102	GLY	C-N-CA	8.53	137.06	121.70
1	A	65	ASP	O-C-N	-8.38	112.41	122.96
1	B	132	ALA	CA-C-N	8.31	133.90	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	132	ALA	C-N-CA	8.31	133.90	120.60
1	B	99	GLU	CA-C-N	8.22	134.54	123.20
1	B	99	GLU	C-N-CA	8.22	134.54	123.20
1	C	102	GLY	O-C-N	-8.14	109.98	123.00
1	A	100	SER	N-CA-C	-8.06	88.43	111.00
1	B	119	GLY	N-CA-C	7.71	124.76	112.58
1	A	100	SER	N-CA-CB	7.69	123.57	110.50
1	C	101	ALA	N-CA-CB	-7.64	98.95	110.40
1	C	100	SER	CA-C-N	7.57	135.33	121.70
1	C	100	SER	C-N-CA	7.57	135.33	121.70
1	B	64	ASP	CA-C-O	7.37	128.05	120.24
1	C	56	GLY	N-CA-C	7.23	121.16	110.60
1	D	132	ALA	CA-C-N	7.09	135.09	121.54
1	D	132	ALA	C-N-CA	7.09	135.09	121.54
1	A	173	LEU	CA-C-N	7.08	130.89	120.90
1	A	173	LEU	C-N-CA	7.08	130.89	120.90
1	D	102	GLY	O-C-N	-7.05	111.72	123.00
1	A	100	SER	CA-CB-OG	6.93	124.96	111.10
1	B	120	HIS	CA-C-N	6.89	130.62	120.90
1	B	120	HIS	C-N-CA	6.89	130.62	120.90
1	A	65	ASP	CA-C-N	-6.84	109.39	121.70
1	A	65	ASP	C-N-CA	-6.84	109.39	121.70
1	B	64	ASP	CB-CA-C	6.81	121.03	110.14
1	B	64	ASP	O-C-N	-6.73	115.39	123.27
1	B	102	GLY	O-C-N	-6.68	112.31	123.00
1	B	81	ALA	N-CA-C	6.49	119.65	110.23
1	B	148	LYS	CB-CA-C	6.49	121.06	110.22
1	A	99	GLU	O-C-N	-6.45	113.56	122.46
1	A	132	ALA	CA-C-N	6.44	133.84	121.54
1	A	132	ALA	C-N-CA	6.44	133.84	121.54
1	A	104	HIS	N-CA-CB	6.42	119.51	109.69
1	C	99	GLU	CA-C-O	6.38	127.23	119.38
1	B	159	ASP	N-CA-C	6.37	119.90	111.75
1	D	118	MET	CA-C-N	6.35	126.78	120.31
1	D	118	MET	C-N-CA	6.35	126.78	120.31
1	B	173	LEU	CA-C-N	6.26	129.76	120.87
1	B	173	LEU	C-N-CA	6.26	129.76	120.87
1	B	133	ASP	N-CA-C	6.21	119.95	112.38
1	A	102	GLY	O-C-N	-6.18	113.11	123.00
1	C	158	GLU	CA-C-N	6.17	129.68	120.31
1	C	158	GLU	C-N-CA	6.17	129.68	120.31
1	C	159	ASP	N-CA-C	6.13	118.93	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	104	HIS	N-CA-C	-6.12	101.25	110.24
1	B	63	SER	CA-C-N	-6.03	114.27	122.77
1	B	63	SER	C-N-CA	-6.03	114.27	122.77
1	B	118	MET	CA-C-N	-5.99	116.13	122.30
1	B	118	MET	C-N-CA	-5.99	116.13	122.30
1	D	99	GLU	CA-C-O	5.98	126.73	119.31
1	D	120	HIS	N-CA-C	5.95	123.47	110.80
1	B	170	ASP	N-CA-CB	-5.93	101.25	109.97
1	B	73	SER	CB-CA-C	5.88	120.22	111.17
1	A	166	HIS	N-CA-C	5.86	119.08	110.59
1	C	179	ASN	N-CA-CB	-5.79	103.50	112.30
1	B	104	HIS	N-CA-CB	5.78	118.54	109.69
1	D	72	ILE	N-CA-C	5.77	116.19	108.11
1	B	98	PHE	N-CA-C	5.77	119.63	112.24
1	B	133	ASP	N-CA-CB	-5.69	100.64	110.32
1	B	173	LEU	N-CA-C	5.65	122.84	110.80
1	C	133	ASP	N-CA-CB	-5.65	101.80	110.16
1	A	106	ASN	CA-C-N	5.61	125.98	119.47
1	A	106	ASN	C-N-CA	5.61	125.98	119.47
1	C	64	ASP	CB-CA-C	5.60	119.41	109.72
1	C	72	ILE	N-CA-C	5.58	115.98	108.17
1	B	135	LYS	N-CA-C	5.56	118.76	110.14
1	A	173	LEU	N-CA-C	5.53	122.59	110.80
1	B	101	ALA	CA-C-N	5.53	131.65	121.70
1	B	101	ALA	C-N-CA	5.53	131.65	121.70
1	D	104	HIS	N-CA-CB	5.46	117.95	109.48
1	B	103	GLY	N-CA-C	5.46	129.14	113.30
1	A	104	HIS	CB-CA-C	-5.46	101.39	109.90
1	A	135	LYS	N-CA-C	5.44	118.45	109.85
1	D	84	GLY	N-CA-C	-5.43	104.15	111.54
1	C	100	SER	N-CA-CB	-5.37	99.80	110.64
1	C	104	HIS	N-CA-CB	5.33	117.74	109.48
1	D	99	GLU	N-CA-C	-5.33	106.29	112.89
1	A	169	ALA	CA-C-N	5.31	128.30	120.82
1	A	169	ALA	C-N-CA	5.31	128.30	120.82
1	D	104	HIS	CA-CB-CG	5.28	119.08	113.80
1	B	100	SER	CA-C-N	5.27	131.18	121.70
1	B	100	SER	C-N-CA	5.27	131.18	121.70
1	C	87	ILE	N-CA-CB	5.19	116.92	111.00
1	A	98	PHE	N-CA-C	5.19	118.75	111.74
1	A	100	SER	CA-C-O	-5.18	111.99	120.80
1	B	158	GLU	CA-C-N	5.16	127.92	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	158	GLU	C-N-CA	5.16	127.92	120.38
1	A	148	LYS	CD-CE-NZ	-5.14	95.45	111.90
1	D	51	GLU	N-CA-C	5.13	119.40	113.20
1	B	78	ARG	CA-C-N	-5.09	114.33	119.83
1	B	78	ARG	C-N-CA	-5.09	114.33	119.83
1	C	185	VAL	N-CA-C	5.08	117.15	108.86
1	C	81	ALA	N-CA-C	5.06	117.63	110.50

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	GLY	Peptide
1	A	64	ASP	Mainchain,Peptide
1	A	99	GLU	Peptide
1	B	101	ALA	Peptide
1	B	102	GLY	Peptide
1	B	120	HIS	Sidechain
1	B	63	SER	Peptide
1	C	101	ALA	Peptide
1	C	102	GLY	Peptide
1	C	64	ASP	Peptide
1	C	95	ARG	Sidechain
1	D	101	ALA	Peptide
1	D	102	GLY	Peptide
1	D	119	GLY	Peptide
1	D	150	GLY	Mainchain
1	D	99	GLU	Peptide

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	1136	0	1077	37	0
1	B	1136	0	1076	26	0
1	C	1136	0	1076	27	0
1	D	1136	0	1075	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	3	0	0	0	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	86	0	0	7	0
4	B	84	0	0	8	0
4	C	70	0	0	4	0
4	D	67	0	0	4	0
All	All	4865	0	4304	118	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 13.

All (118) 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:65:ASP:CB	1:A:66:GLU:HB3	1.81	1.11
1:A:65:ASP:HB2	1:A:66:GLU:HB3	1.40	1.01
1:B:100:SER:HB3	4:B:1330:HOH:O	1.59	1.00
4:A:1344:HOH:O	1:D:101:ALA:HB2	1.75	0.87
1:A:100:SER:H	1:A:101:ALA:CA	1.88	0.87
1:B:99:GLU:HB3	1:C:99:GLU:OE2	1.81	0.81
1:C:100:SER:CB	4:C:1388:HOH:O	2.29	0.80
1:B:97:ASP:HB2	4:B:1379:HOH:O	1.81	0.80
1:D:65:ASP:HB3	1:D:66:GLU:HB3	1.63	0.80
1:A:65:ASP:HB3	1:A:66:GLU:HB3	1.64	0.79
1:C:100:SER:HB3	4:C:1388:HOH:O	1.82	0.79
1:A:100:SER:H	1:A:101:ALA:HA	1.46	0.78
1:D:133:ASP:HB2	1:D:135:LYS:H	1.49	0.77
1:B:168:GLN:CD	4:B:1406:HOH:O	2.26	0.77
1:D:86:HIS:ND1	1:D:104:HIS:NE2	2.34	0.74
1:A:156:LEU:HD22	1:A:191:GLY:HA3	1.68	0.74
1:C:64:ASP:HA	1:C:65:ASP:HB3	1.70	0.73
1:C:50:ARG:HG2	1:C:96:PRO:O	1.91	0.71
1:D:62:GLU:HG3	1:D:147:LEU:HD12	1.76	0.67
1:A:97:ASP:HB2	4:A:1343:HOH:O	1.94	0.67
1:D:86:HIS:ND1	1:D:104:HIS:CE1	2.63	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:ASN:HD21	1:D:170:ASP:HB3	1.61	0.66
1:A:100:SER:N	1:A:101:ALA:HA	2.11	0.66
1:D:157:ASP:O	1:D:191:GLY:HA3	1.95	0.66
1:D:86:HIS:CE1	1:D:104:HIS:CE1	2.84	0.66
1:B:165:ILE:HB	1:B:185:VAL:HB	1.78	0.65
1:A:64:ASP:HA	1:A:65:ASP:HB3	1.78	0.65
1:A:65:ASP:HB2	1:A:66:GLU:CB	2.22	0.63
1:A:84:GLY:HA2	1:A:127:ASN:HD22	1.65	0.62
1:A:108:LEU:HD11	1:A:152:LYS:HE2	1.82	0.62
1:A:62:GLU:HG2	4:A:1349:HOH:O	2.02	0.59
1:D:78:ARG:HD3	4:D:1349:HOH:O	2.02	0.59
1:D:112:HIS:HB2	1:D:121:HIS:CE1	2.37	0.59
1:C:65:ASP:HB2	1:C:66:GLU:HB3	1.84	0.59
1:A:65:ASP:HB2	1:A:66:GLU:OE1	2.01	0.59
1:D:99:GLU:O	1:D:101:ALA:HA	2.03	0.58
1:A:64:ASP:HA	1:A:65:ASP:CB	2.33	0.58
1:C:127:ASN:HD21	1:C:170:ASP:H	1.50	0.58
1:A:94:VAL:HB	1:A:100:SER:HB3	1.85	0.57
1:B:62:GLU:HG2	4:B:1411:HOH:O	2.03	0.57
1:B:94:VAL:HB	1:B:100:SER:HB2	1.85	0.57
1:C:99:GLU:O	1:C:101:ALA:HA	2.05	0.57
1:A:100:SER:HB3	4:A:1355:HOH:O	2.05	0.57
1:C:64:ASP:HA	1:C:65:ASP:CB	2.32	0.56
1:B:110:LYS:HD2	4:B:1408:HOH:O	2.04	0.56
1:B:99:GLU:O	1:B:101:ALA:HA	2.05	0.56
1:A:89:GLU:OE2	1:A:103:GLY:HA3	2.06	0.55
1:A:65:ASP:CB	1:A:66:GLU:CB	2.71	0.55
1:A:156:LEU:HD22	1:A:191:GLY:CA	2.34	0.55
1:C:92:SER:HB3	1:C:101:ALA:H	1.72	0.54
1:C:89:GLU:OE2	1:C:103:GLY:HA3	2.08	0.54
1:B:116:ASN:HB3	1:B:119:GLY:HA3	1.90	0.54
1:B:110:LYS:HE3	4:B:1408:HOH:O	2.08	0.54
1:D:62:GLU:HB2	4:D:1388:HOH:O	2.07	0.54
1:C:178:GLY:O	1:C:179:ASN:CB	2.53	0.53
1:B:98:PHE:C	1:B:100:SER:H	2.14	0.53
1:C:98:PHE:C	1:C:100:SER:H	2.15	0.53
1:A:113:GLY:O	1:A:120:HIS:HB3	2.09	0.53
1:C:102:GLY:O	1:C:183:ARG:NH1	2.41	0.53
1:B:84:GLY:HA2	1:B:127:ASN:HD22	1.75	0.51
1:A:99:GLU:O	1:A:101:ALA:HA	2.09	0.51
1:C:90:LYS:HD3	1:C:101:ALA:CB	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:GLU:CG	4:B:1411:HOH:O	2.56	0.51
1:C:128:LEU:HB3	1:C:136:VAL:HG21	1.93	0.50
1:B:89:GLU:OE2	1:B:103:GLY:HA3	2.12	0.50
1:A:43:HIS:CD2	4:A:1369:HOH:O	2.64	0.50
1:A:43:HIS:HE1	4:A:1363:HOH:O	1.95	0.50
1:B:133:ASP:HB3	1:B:135:LYS:H	1.77	0.49
1:A:99:GLU:OE2	4:A:1374:HOH:O	2.20	0.49
1:D:127:ASN:HD21	1:D:170:ASP:CB	2.25	0.49
1:C:80:GLY:HA2	1:C:130:VAL:O	2.13	0.49
1:D:149:LYS:HG3	1:D:149:LYS:O	2.12	0.48
1:D:133:ASP:HB2	1:D:135:LYS:N	2.24	0.48
1:B:95:ARG:HB3	1:B:96:PRO:HA	1.95	0.48
1:B:127:ASN:HD21	1:B:170:ASP:H	1.62	0.48
1:A:82:SER:HB2	1:A:169:ALA:HB2	1.95	0.48
1:B:110:LYS:CE	4:B:1408:HOH:O	2.62	0.48
1:A:109:ASN:HB2	1:D:109:ASN:OD1	2.14	0.48
1:A:50:ARG:CZ	1:A:184:ILE:HG22	2.43	0.47
1:C:157:ASP:O	1:C:191:GLY:HA3	2.13	0.47
1:D:152:LYS:HG2	1:D:153:LEU:HD23	1.96	0.47
1:A:63:SER:HB3	1:A:67:GLY:O	2.14	0.47
1:D:88:TYR:CZ	1:D:104:HIS:HD2	2.32	0.47
1:D:90:LYS:HD3	1:D:101:ALA:CB	2.44	0.47
1:C:95:ARG:HG2	1:C:98:PHE:CE1	2.49	0.46
1:D:127:ASN:HD21	1:D:170:ASP:H	1.62	0.46
1:A:70:ILE:HD13	1:A:163:PHE:HE1	1.79	0.46
1:C:63:SER:HB3	1:C:67:GLY:O	2.15	0.46
1:D:156:LEU:O	1:D:156:LEU:HD13	2.16	0.46
1:B:102:GLY:O	1:B:183:ARG:NH1	2.47	0.45
1:C:106:ASN:CG	1:C:121:HIS:HD2	2.25	0.45
1:C:151:SER:HA	4:C:1368:HOH:O	2.15	0.45
1:D:62:GLU:N	4:D:1388:HOH:O	2.29	0.45
1:C:65:ASP:HA	1:C:66:GLU:HA	1.76	0.44
1:D:66:GLU:N	1:D:66:GLU:OE1	2.51	0.43
1:A:41:PHE:CE2	1:A:61:LYS:HB3	2.54	0.43
1:A:65:ASP:HB2	1:A:66:GLU:CD	2.43	0.43
1:D:85:PHE:HB2	1:D:128:LEU:HG	2.00	0.43
1:A:65:ASP:HA	1:A:66:GLU:HA	1.60	0.42
1:A:127:ASN:HD21	1:A:170:ASP:H	1.67	0.42
1:D:168:GLN:HE21	1:D:168:GLN:HB2	1.73	0.42
1:B:72:ILE:HD11	1:B:165:ILE:HD11	2.02	0.42
1:D:166:HIS:CG	1:D:180:SER:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:HIS:HB3	1:C:180:SER:O	2.20	0.41
1:D:89:GLU:OE2	1:D:103:GLY:HA3	2.20	0.41
1:B:84:GLY:HA2	1:B:127:ASN:ND2	2.35	0.41
1:B:127:ASN:HD21	1:B:170:ASP:CB	2.34	0.41
1:C:127:ASN:ND2	1:C:170:ASP:H	2.18	0.41
1:C:90:LYS:CE	4:C:1330:HOH:O	2.68	0.41
1:B:88:TYR:CE1	1:B:164:ILE:HB	2.56	0.41
1:A:137:ASP:OD1	1:A:137:ASP:C	2.60	0.41
1:B:64:ASP:HA	1:B:65:ASP:HA	1.67	0.41
1:B:99:GLU:HA	1:B:183:ARG:NH1	2.36	0.41
1:A:94:VAL:HB	1:A:100:SER:CB	2.49	0.41
1:D:117:PRO:C	1:D:119:GLY:H	2.28	0.41
1:C:112:HIS:HB2	1:C:121:HIS:CE1	2.55	0.41
1:D:62:GLU:HG2	4:D:1371:HOH:O	2.20	0.40
1:A:99:GLU:N	1:A:100:SER:OG	2.55	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	150/175 (86%)	138 (92%)	10 (7%)	2 (1%)	9	5
1	B	150/175 (86%)	139 (93%)	10 (7%)	1 (1%)	18	14
1	C	150/175 (86%)	137 (91%)	13 (9%)	0	100	100
1	D	150/175 (86%)	137 (91%)	11 (7%)	2 (1%)	9	5
All	All	600/700 (86%)	551 (92%)	44 (7%)	5 (1%)	16	11

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	SER
1	D	120	HIS
1	A	133	ASP
1	D	62	GLU
1	B	103	GLY

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%)	106 (88%)	14 (12%)	5	3
1	B	120/143 (84%)	103 (86%)	17 (14%)	3	2
1	C	120/143 (84%)	102 (85%)	18 (15%)	3	1
1	D	120/143 (84%)	109 (91%)	11 (9%)	8	5
All	All	480/572 (84%)	420 (88%)	60 (12%)	4	2

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	45	VAL
1	B	62	GLU
1	B	63	SER
1	B	66	GLU
1	B	82	SER
1	B	99	GLU
1	B	100	SER
1	B	108	LEU
1	B	110	LYS
1	B	120	HIS
1	B	133	ASP
1	B	149	LYS
1	B	156	LEU
1	B	158	GLU
1	B	159	ASP
1	B	168	GLN
1	B	190	LEU

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Mol	Chain	Res	Type
1	A	45	VAL
1	A	58	ILE
1	A	61	LYS
1	A	65	ASP
1	A	66	GLU
1	A	73	SER
1	A	82	SER
1	A	108	LEU
1	A	110	LYS
1	A	133	ASP
1	A	152	LYS
1	A	156	LEU
1	A	167	GLU
1	A	190	LEU
1	C	45	VAL
1	C	48	VAL
1	C	61	LYS
1	C	62	GLU
1	C	82	SER
1	C	95	ARG
1	C	100	SER
1	C	110	LYS
1	C	118	MET
1	C	136	VAL
1	C	140	MET
1	C	149	LYS
1	C	151	SER
1	C	152	LYS
1	C	156	LEU
1	C	159	ASP
1	C	184	ILE
1	C	190	LEU
1	D	45	VAL
1	D	48	VAL
1	D	66	GLU
1	D	100	SER
1	D	120	HIS
1	D	146	SER
1	D	149	LYS
1	D	167	GLU
1	D	168	GLN
1	D	179	ASN

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Mol	Chain	Res	Type
1	D	180	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	43	HIS
1	B	86	HIS
1	B	116	ASN
1	B	127	ASN
1	B	179	ASN
1	A	43	HIS
1	A	127	ASN
1	C	44	HIS
1	C	127	ASN
1	D	127	ASN
1	D	168	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 14 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	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	65:ASP	C	66:GLU	N	1.65

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	152/175 (86%)	0.55	8 (5%) 32 31	16, 25, 35, 55	2 (1%)
1	B	152/175 (86%)	0.57	8 (5%) 32 31	16, 24, 37, 50	0
1	C	152/175 (86%)	0.62	12 (7%) 18 17	16, 26, 39, 46	0
1	D	152/175 (86%)	0.67	9 (5%) 28 27	14, 26, 39, 45	0
All	All	608/700 (86%)	0.60	37 (6%) 27 26	14, 25, 39, 55	2 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	65	ASP	8.8
1	B	65	ASP	8.8
1	B	64	ASP	6.9
1	C	64	ASP	4.9
1	D	64	ASP	4.4
1	A	63	SER	4.2
1	D	150	GLY	4.1
1	A	64	ASP	4.1
1	D	152	LYS	3.8
1	C	101	ALA	3.4
1	B	100	SER	3.3
1	A	101	ALA	3.3
1	C	162	ALA	3.1
1	B	190	LEU	3.1
1	D	65	ASP	3.1
1	A	191	GLY	3.0
1	C	65	ASP	3.0
1	C	100	SER	2.9
1	D	100	SER	2.7
1	D	101	ALA	2.6
1	B	131	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	102	GLY	2.5
1	C	66	GLU	2.4
1	B	101	ALA	2.4
1	C	40	ALA	2.4
1	B	63	SER	2.4
1	C	133	ASP	2.4
1	C	191	GLY	2.3
1	A	100	SER	2.2
1	D	117	PRO	2.2
1	D	40	ALA	2.2
1	C	158	GLU	2.1
1	A	133	ASP	2.1
1	D	120	HIS	2.1
1	C	150	GLY	2.1
1	B	119	GLY	2.1
1	A	102	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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($\text{\AA}^2$)	Q<0.9
2	CU	D	1177	1/1	0.95	0.09	29,29,29,29	0
3	ZN	A	1331	1/1	0.96	0.07	41,41,41,41	0
2	CU	B	1171	1/1	0.97	0.04	27,27,27,27	0
2	CU	A	1173	1/1	0.97	0.06	27,27,27,27	0
3	ZN	C	1328	1/1	0.98	0.05	39,39,39,39	0
3	ZN	B	1329	1/1	0.99	0.09	39,39,39,39	0
3	ZN	A	1174	1/1	0.99	0.03	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CU	C	1175	1/1	0.99	0.04	34,34,34,34	0
3	ZN	C	1176	1/1	0.99	0.04	23,23,23,23	0
3	ZN	B	1326	1/1	0.99	0.04	26,26,26,26	0
3	ZN	D	1178	1/1	0.99	0.03	22,22,22,22	0
3	ZN	D	1330	1/1	0.99	0.03	40,40,40,40	0
3	ZN	A	1327	1/1	1.00	0.04	26,26,26,26	0
3	ZN	B	1172	1/1	1.00	0.05	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.