



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 04:35 AM UTC

PDB ID : 1HL5 / pdb_00001hl5
Title : The Structure of Holo Type Human Cu, Zn Superoxide Dismutase
Authors : Strange, R.W.; Antonyuk, S.; Hough, M.A.; Doucette, P.; Rodriguez, J.; Hart, P.J.; Hayward, L.J.; Valentine, J.S.; Hasnain, S.S.
Deposited on : 2003-03-13
Resolution : 1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

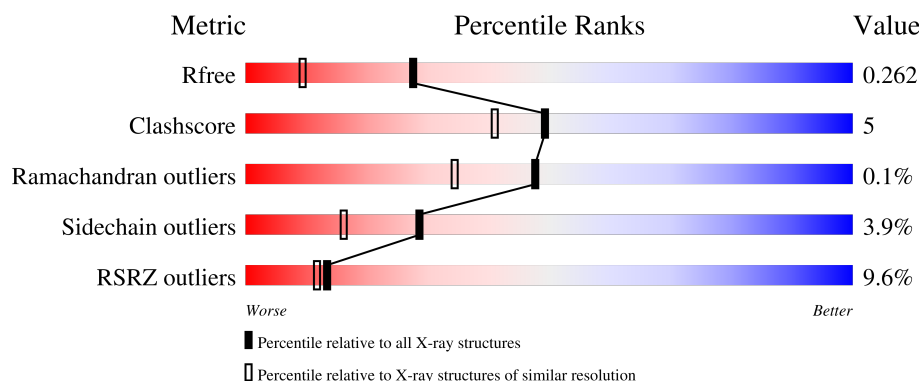
1 Overall quality at a glance

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	153	% 92% 8%
1	B	153	3% 88% 11% ..
1	C	153	2% 95% 5%
1	D	153	% 93% 5% ..
1	E	153	% 90% 8% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	153	 % 86% 7% • 5%
1	G	153	 19% 78% 18% • •
1	H	153	 % 96% • •
1	I	153	 % 93% 7%
1	J	153	 % 93% 7% •
1	K	153	 3% 92% 8% •
1	L	153	 % 93% 5% • •
1	M	153	 3% 88% 10% • •
1	N	153	 % 90% 9% •
1	O	153	 16% 76% 20% •
1	P	153	 87% 86% 12% •
1	Q	153	 6% 81% 14% 5% •
1	S	153	 24% 82% 18%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21585 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	0	0
			1110	679	203	224	4			
1	B	153	Total	C	N	O	S	0	0	0
			1110	679	203	224	4			
1	C	153	Total	C	N	O	S	0	0	0
			1109	679	202	224	4			
1	D	153	Total	C	N	O	S	0	0	0
			1094	672	199	219	4			
1	E	151	Total	C	N	O	S	0	0	0
			1082	669	195	214	4			
1	F	145	Total	C	N	O	S	0	0	1
			1031	634	187	206	4			
1	G	153	Total	C	N	O	S	0	0	0
			1110	679	203	224	4			
1	H	153	Total	C	N	O	S	0	0	0
			1110	679	203	224	4			
1	I	153	Total	C	N	O	S	0	0	0
			1110	679	203	224	4			
1	J	153	Total	C	N	O	S	0	0	0
			1102	675	199	224	4			
1	K	153	Total	C	N	O	S	0	0	0
			1106	678	201	223	4			
1	L	152	Total	C	N	O	S	0	0	0
			1096	672	198	222	4			
1	M	152	Total	C	N	O	S	0	0	1
			1075	660	194	217	4			
1	N	153	Total	C	N	O	S	0	0	0
			1110	679	203	224	4			
1	O	153	Total	C	N	O	S	0	0	0
			1109	679	203	223	4			
1	P	153	Total	C	N	O	S	0	0	0
			1101	674	201	222	4			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	153	Total	C	N	O	S	0	0	0
			1110	679	203	224	4			
1	S	153	Total	C	N	O	S	0	0	0
			1108	678	202	224	4			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cu	0	0
			1	1		
2	B	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		
2	E	1	Total	Cu	0	0
			1	1		
2	F	1	Total	Cu	0	0
			1	1		
2	G	1	Total	Cu	0	0
			1	1		
2	H	1	Total	Cu	0	0
			1	1		
2	I	1	Total	Cu	0	0
			1	1		
2	J	1	Total	Cu	0	0
			1	1		
2	K	1	Total	Cu	0	0
			1	1		
2	L	1	Total	Cu	0	0
			1	1		
2	M	1	Total	Cu	0	0
			1	1		
2	N	1	Total	Cu	0	0
			1	1		
2	O	1	Total	Cu	0	0
			1	1		
2	P	1	Total	Cu	0	0
			1	1		
2	Q	1	Total	Cu	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	S	1	Total	Cu	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		
3	G	1	Total	Zn	0	0
			1	1		
3	H	1	Total	Zn	0	0
			1	1		
3	I	1	Total	Zn	0	0
			1	1		
3	J	1	Total	Zn	0	0
			1	1		
3	K	1	Total	Zn	0	0
			1	1		
3	L	1	Total	Zn	0	0
			1	1		
3	M	1	Total	Zn	0	0
			1	1		
3	N	1	Total	Zn	0	0
			1	1		
3	O	1	Total	Zn	0	0
			1	1		
3	P	1	Total	Zn	0	0
			1	1		
3	Q	1	Total	Zn	0	0
			1	1		
3	S	1	Total	Zn	0	0
			1	1		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total 1	Ca 1	0	0
4	D	1	Total 1	Ca 1	0	0
4	O	1	Total 1	Ca 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	113	Total 113	O 113	0	0
5	B	152	Total 152	O 152	0	0
5	C	144	Total 144	O 144	0	0
5	D	107	Total 107	O 107	0	0
5	E	114	Total 114	O 114	0	0
5	F	94	Total 94	O 94	0	0
5	G	43	Total 43	O 43	0	0
5	H	118	Total 118	O 118	0	0
5	I	141	Total 141	O 141	0	0
5	J	133	Total 133	O 133	0	0
5	K	148	Total 148	O 148	0	0
5	L	115	Total 115	O 115	0	0
5	M	99	Total 99	O 99	0	0
5	N	90	Total 90	O 90	0	0
5	O	50	Total 50	O 50	0	0
5	P	2	Total 2	O 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	Q	83	Total	O	0	0
			83	83		
5	S	17	Total	O	0	0
			17	17		

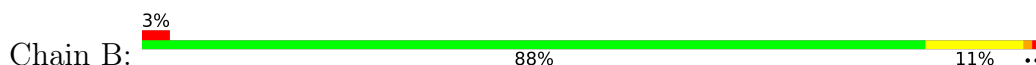
3 Residue-property plots

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



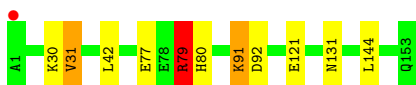
- Molecule 1: SUPEROXIDE DISMUTASE



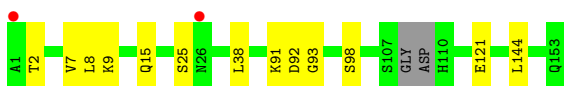
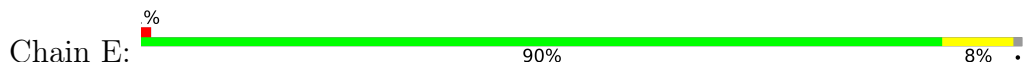
- Molecule 1: SUPEROXIDE DISMUTASE



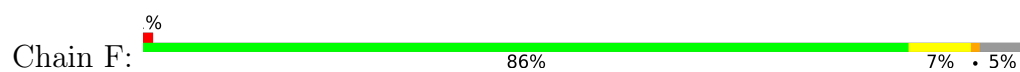
- Molecule 1: SUPEROXIDE DISMUTASE



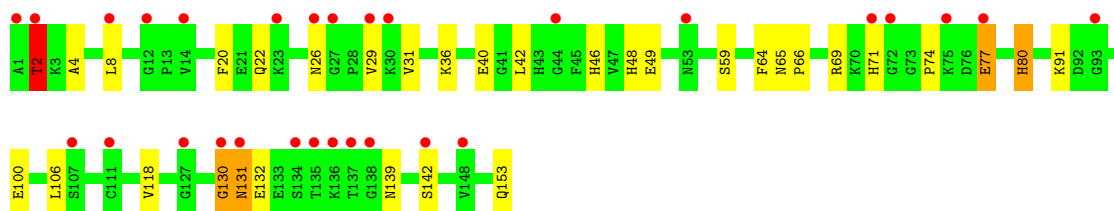
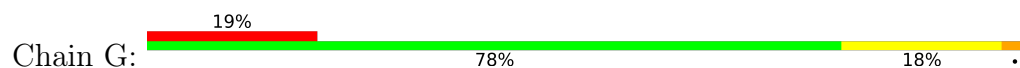
- Molecule 1: SUPEROXIDE DISMUTASE



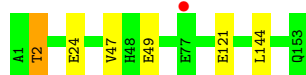
- Molecule 1: SUPEROXIDE DISMUTASE



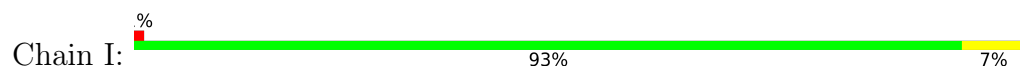
• Molecule 1: SUPEROXIDE DISMUTASE



• Molecule 1: SUPEROXIDE DISMUTASE



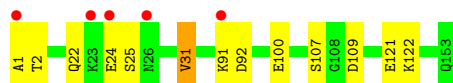
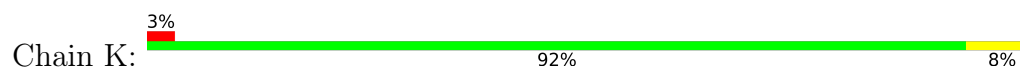
• Molecule 1: SUPEROXIDE DISMUTASE



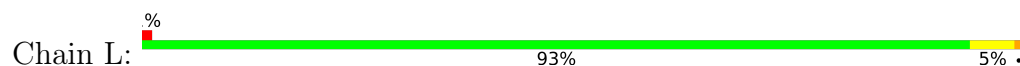
• Molecule 1: SUPEROXIDE DISMUTASE



• Molecule 1: SUPEROXIDE DISMUTASE

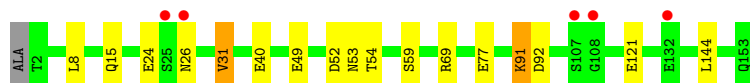
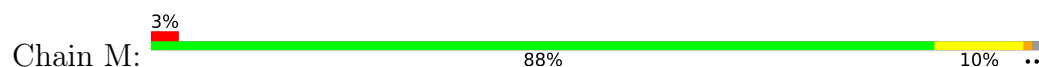


• Molecule 1: SUPEROXIDE DISMUTASE





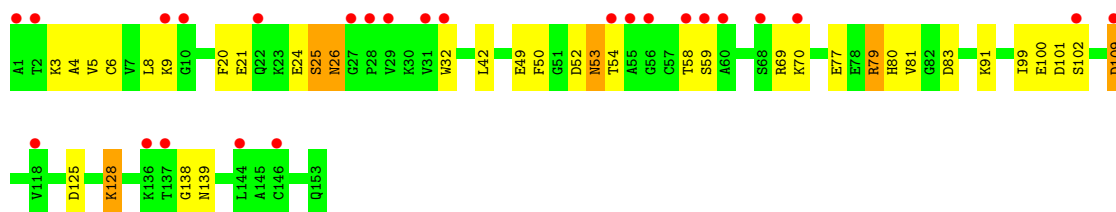
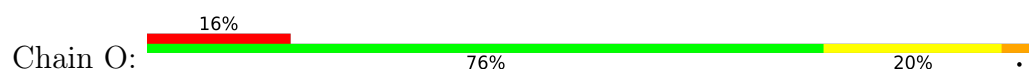
● Molecule 1: SUPEROXIDE DISMUTASE



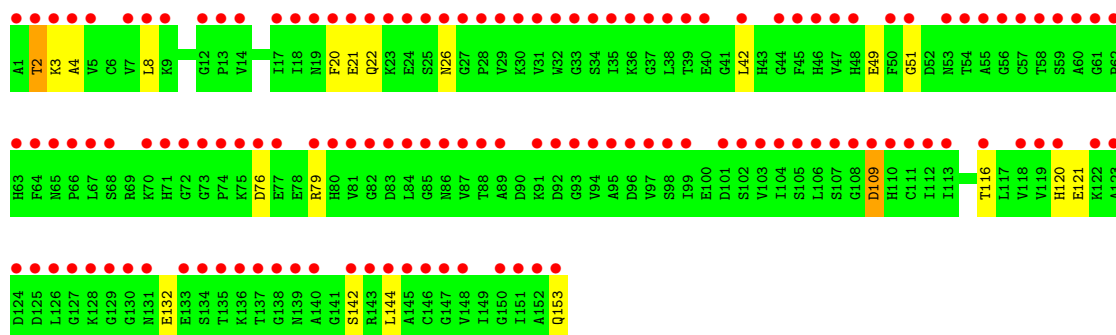
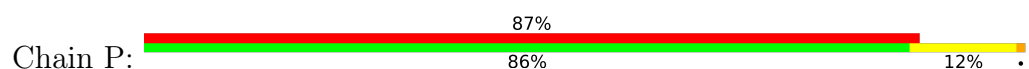
● Molecule 1: SUPEROXIDE DISMUTASE



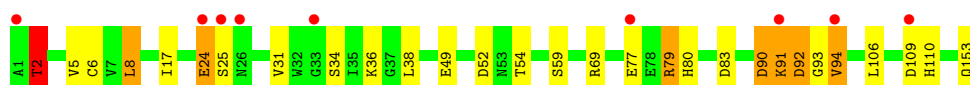
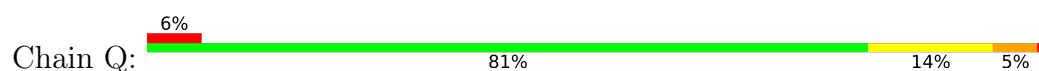
● Molecule 1: SUPEROXIDE DISMUTASE



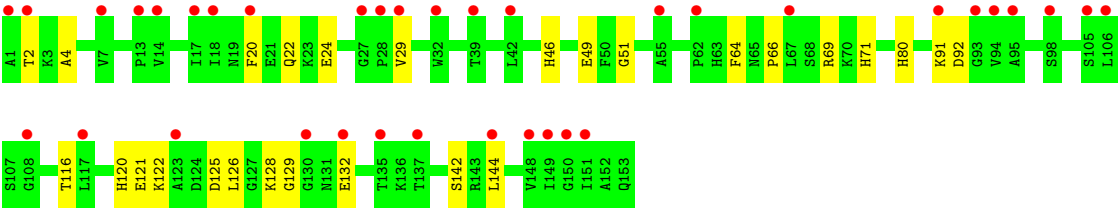
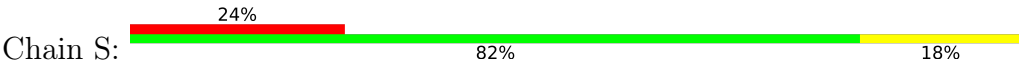
● Molecule 1: SUPEROXIDE DISMUTASE



● Molecule 1: SUPEROXIDE DISMUTASE



● Molecule 1: SUPEROXIDE DISMUTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.87Å 172.38Å 112.45Å 90.00° 93.45° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 50.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-1.80) 98.6 (50.00-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.185 , 0.222 0.237 , 0.262	Depositor DCC
R_{free} test set	13374 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.5	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	21585	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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: ZN, CA, CU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.78	0/1128	1.10	1/1520 (0.1%)
1	B	0.89	0/1128	1.11	2/1520 (0.1%)
1	C	0.90	0/1127	1.10	1/1519 (0.1%)
1	D	0.80	0/1112	1.10	3/1501 (0.2%)
1	E	0.77	0/1099	1.03	0/1482
1	F	0.73	0/1048	1.08	1/1413 (0.1%)
1	G	0.63	0/1128	1.12	5/1520 (0.3%)
1	H	0.78	1/1128 (0.1%)	1.07	2/1520 (0.1%)
1	I	0.87	0/1128	1.07	0/1520
1	J	0.86	0/1120	1.08	0/1512
1	K	0.90	0/1124	1.11	2/1515 (0.1%)
1	L	0.74	0/1114	1.05	2/1503 (0.1%)
1	M	0.78	0/1092	1.08	4/1471 (0.3%)
1	N	0.73	0/1128	1.08	2/1520 (0.1%)
1	O	0.67	0/1127	1.06	3/1520 (0.2%)
1	P	0.31	0/1118	0.92	4/1506 (0.3%)
1	Q	0.78	0/1128	1.12	4/1520 (0.3%)
1	S	0.43	0/1126	0.98	4/1518 (0.3%)
All	All	0.76	1/20103 (0.0%)	1.07	40/27100 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	47	VAL	CA-CB	-5.26	1.48	1.54

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	77	GLU	N-CA-C	-9.75	101.89	113.88
1	P	153	GLN	OE1-CD-NE2	-9.31	113.29	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	129	GLY	N-CA-C	8.73	124.27	114.67
1	G	130	GLY	N-CA-C	-7.71	104.57	111.67
1	P	49	GLU	N-CA-C	7.61	119.22	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1110	0	1077	6	0
1	B	1110	0	1077	11	1
1	C	1109	0	1072	7	0
1	D	1094	0	1041	7	0
1	E	1082	0	1031	10	0
1	F	1031	0	982	8	0
1	G	1110	0	1077	21	0
1	H	1110	0	1077	1	0
1	I	1110	0	1077	8	0
1	J	1102	0	1049	20	0
1	K	1106	0	1068	7	0
1	L	1096	0	1044	6	0
1	M	1075	0	1009	11	2
1	N	1110	0	1077	15	0
1	O	1109	0	1077	32	0
1	P	1101	0	1059	9	0
1	Q	1110	0	1077	23	0
1	S	1108	0	1070	25	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
2	Q	1	0	0	0	0
2	S	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	S	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	O	1	0	0	0	0
5	A	113	0	0	2	0
5	B	152	0	0	4	0
5	C	144	0	0	5	1
5	D	107	0	0	1	0
5	E	114	0	0	0	0
5	F	94	0	0	1	0
5	G	43	0	0	4	0
5	H	118	0	0	0	1
5	I	141	0	0	1	0
5	J	133	0	0	4	0
5	K	148	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	115	0	0	5	0
5	M	99	0	0	3	0
5	N	90	0	0	7	0
5	O	50	0	0	10	0
5	P	2	0	0	0	0
5	Q	83	0	0	4	0
5	S	17	0	0	3	0
All	All	21585	0	19041	208	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 208 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:96:ASP:HB3	5:I:2092:HOH:O	1.27	1.25
1:A:96:ASP:HB3	5:A:2072:HOH:O	1.42	1.16
1:O:125:ASP:O	1:O:128:LYS:HE2	1.47	1.14
1:J:153:GLN:O	1:S:92:ASP:OD1	1.68	1.10
1:B:53:ASN:OD1	5:B:2071:HOH:O	1.76	1.04

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:54:THR:O	1:S:132:GLU:OE2[1_456]	1.86	0.34
1:B:122:LYS:NZ	1:M:40:GLU:OE2[2_546]	1.92	0.28
5:C:2120:HOH:O	5:H:2064:HOH:O[1_554]	2.06	0.14

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	151/153 (99%)	150 (99%)	1 (1%)	0	100	100
1	B	151/153 (99%)	150 (99%)	1 (1%)	0	100	100
1	C	151/153 (99%)	150 (99%)	1 (1%)	0	100	100
1	D	151/153 (99%)	149 (99%)	2 (1%)	0	100	100
1	E	147/153 (96%)	146 (99%)	1 (1%)	0	100	100
1	F	141/153 (92%)	140 (99%)	1 (1%)	0	100	100
1	G	151/153 (99%)	146 (97%)	4 (3%)	1 (1%)	18	8
1	H	151/153 (99%)	149 (99%)	2 (1%)	0	100	100
1	I	151/153 (99%)	148 (98%)	3 (2%)	0	100	100
1	J	151/153 (99%)	150 (99%)	1 (1%)	0	100	100
1	K	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
1	L	150/153 (98%)	149 (99%)	1 (1%)	0	100	100
1	M	149/153 (97%)	148 (99%)	1 (1%)	0	100	100
1	N	151/153 (99%)	151 (100%)	0	0	100	100
1	O	151/153 (99%)	146 (97%)	3 (2%)	2 (1%)	9	3
1	P	150/153 (98%)	147 (98%)	3 (2%)	0	100	100
1	Q	151/153 (99%)	146 (97%)	4 (3%)	1 (1%)	18	8
1	S	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
All	All	2700/2754 (98%)	2656 (98%)	40 (2%)	4 (0%)	48	34

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	131	ASN
1	O	25	SER
1	O	26	ASN
1	Q	2	THR

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	118/118 (100%)	112 (95%)	6 (5%)	21	9
1	B	118/118 (100%)	112 (95%)	6 (5%)	21	9
1	C	117/118 (99%)	117 (100%)	0	100	100
1	D	111/118 (94%)	107 (96%)	4 (4%)	31	18
1	E	108/118 (92%)	106 (98%)	2 (2%)	50	41
1	F	107/118 (91%)	101 (94%)	6 (6%)	19	8
1	G	118/118 (100%)	109 (92%)	9 (8%)	12	4
1	H	118/118 (100%)	116 (98%)	2 (2%)	53	45
1	I	118/118 (100%)	116 (98%)	2 (2%)	53	45
1	J	114/118 (97%)	112 (98%)	2 (2%)	51	43
1	K	116/118 (98%)	112 (97%)	4 (3%)	32	20
1	L	114/118 (97%)	112 (98%)	2 (2%)	51	43
1	M	108/118 (92%)	105 (97%)	3 (3%)	38	26
1	N	118/118 (100%)	114 (97%)	4 (3%)	32	20
1	O	118/118 (100%)	109 (92%)	9 (8%)	12	4
1	P	115/118 (98%)	110 (96%)	5 (4%)	26	13
1	Q	118/118 (100%)	107 (91%)	11 (9%)	8	2
1	S	117/118 (99%)	113 (97%)	4 (3%)	32	20
All	All	2071/2124 (98%)	1990 (96%)	81 (4%)	28	16

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	91	LYS
1	Q	59	SER
1	O	109	ASP
1	P	109	ASP
1	Q	90	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	139	ASN
1	Q	110	HIS
1	G	65	ASN
1	G	139	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	15	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 39 ligands modelled in this entry, 39 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	153/153 (100%)	-0.06	2 (1%) 75 75	6, 11, 22, 33	0
1	B	153/153 (100%)	-0.03	4 (2%) 57 57	5, 7, 19, 29	0
1	C	153/153 (100%)	-0.15	3 (1%) 65 65	5, 6, 19, 25	0
1	D	153/153 (100%)	-0.04	1 (0%) 84 85	5, 12, 20, 26	0
1	E	151/153 (98%)	-0.21	2 (1%) 75 75	6, 11, 19, 29	0
1	F	145/153 (94%)	0.11	1 (0%) 84 85	10, 15, 24, 33	0
1	G	153/153 (100%)	1.54	29 (18%) 3 2	15, 21, 35, 42	0
1	H	153/153 (100%)	0.05	1 (0%) 84 85	7, 11, 21, 28	0
1	I	153/153 (100%)	-0.17	2 (1%) 75 75	5, 8, 18, 22	0
1	J	153/153 (100%)	-0.20	2 (1%) 75 75	5, 7, 16, 24	0
1	K	153/153 (100%)	-0.04	5 (3%) 49 49	5, 7, 16, 26	0
1	L	152/153 (99%)	-0.02	1 (0%) 84 85	8, 13, 22, 29	0
1	M	152/153 (99%)	0.07	5 (3%) 49 49	5, 11, 22, 32	0
1	N	153/153 (100%)	0.32	1 (0%) 84 85	6, 14, 25, 31	1 (0%)
1	O	153/153 (100%)	1.16	25 (16%) 4 3	15, 21, 34, 40	0
1	P	153/153 (100%)	3.17	133 (86%) 0 0	50, 62, 66, 69	0
1	Q	153/153 (100%)	0.69	9 (5%) 28 27	5, 14, 26, 36	0
1	S	153/153 (100%)	1.43	36 (23%) 2 1	25, 35, 47, 52	0
All	All	2742/2754 (99%)	0.43	262 (9%) 13 12	5, 13, 54, 69	1 (0%)

The worst 5 of 262 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	1	ALA	7.2
1	P	94	VAL	6.3
1	P	74	PRO	6.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	P	151	ILE	6.2
1	K	1	ALA	5.8

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
3	ZN	P	155	1/1	0.78	0.33	61,61,61,61	0
2	CU	P	154	1/1	0.90	0.23	69,69,69,69	0
3	ZN	G	155	1/1	0.94	0.28	20,20,20,20	0
2	CU	G	154	1/1	0.95	0.27	27,27,27,27	0
4	CA	C	156	1/1	0.95	0.07	37,37,37,37	1
4	CA	D	156	1/1	0.95	0.11	47,47,47,47	0
2	CU	H	154	1/1	0.96	0.20	22,22,22,22	0
2	CU	A	154	1/1	0.96	0.17	17,17,17,17	0
2	CU	S	154	1/1	0.97	0.22	46,46,46,46	0
2	CU	N	154	1/1	0.97	0.18	22,22,22,22	0
3	ZN	O	155	1/1	0.97	0.27	18,18,18,18	0
2	CU	O	154	1/1	0.97	0.21	29,29,29,29	0
2	CU	M	154	1/1	0.97	0.17	23,23,23,23	0
2	CU	Q	154	1/1	0.97	0.15	22,22,22,22	0
2	CU	B	154	1/1	0.98	0.18	15,15,15,15	0
2	CU	C	154	1/1	0.98	0.19	16,16,16,16	0
2	CU	I	154	1/1	0.98	0.17	17,17,17,17	0
2	CU	J	154	1/1	0.98	0.17	15,15,15,15	0
3	ZN	H	155	1/1	0.98	0.23	10,10,10,10	0
3	ZN	N	155	1/1	0.98	0.24	11,11,11,11	0
2	CU	K	154	1/1	0.98	0.20	13,13,13,13	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CU	D	154	1/1	0.98	0.20	21,21,21,21	0
2	CU	E	154	1/1	0.98	0.16	20,20,20,20	0
2	CU	F	154	1/1	0.98	0.17	22,22,22,22	0
4	CA	O	156	1/1	0.98	0.09	44,44,44,44	0
3	ZN	J	155	1/1	0.99	0.23	6,6,6,6	0
3	ZN	M	155	1/1	0.99	0.23	9,9,9,9	0
3	ZN	C	155	1/1	0.99	0.22	5,5,5,5	0
3	ZN	D	155	1/1	0.99	0.22	10,10,10,10	0
3	ZN	F	155	1/1	0.99	0.23	12,12,12,12	0
3	ZN	Q	155	1/1	0.99	0.21	12,12,12,12	0
3	ZN	S	155	1/1	0.99	0.29	27,27,27,27	0
2	CU	L	154	1/1	0.99	0.15	22,22,22,22	0
3	ZN	A	155	1/1	0.99	0.20	8,8,8,8	0
3	ZN	I	155	1/1	0.99	0.22	7,7,7,7	0
3	ZN	B	155	1/1	1.00	0.21	5,5,5,5	0
3	ZN	K	155	1/1	1.00	0.20	5,5,5,5	0
3	ZN	L	155	1/1	1.00	0.20	9,9,9,9	0
3	ZN	E	155	1/1	1.00	0.21	8,8,8,8	0

6.5 Other polymers [i](#)

There are no such residues in this entry.