



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 03:59 pm BST

PDB ID : 6DTK
Title : Heterodimers of FALS mutant SOD enzyme
Authors : Streltsov, V.A.; Nuttall, S.D.; Ganio, K.E.; Roberts, B.
Deposited on : 2018-06-17
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

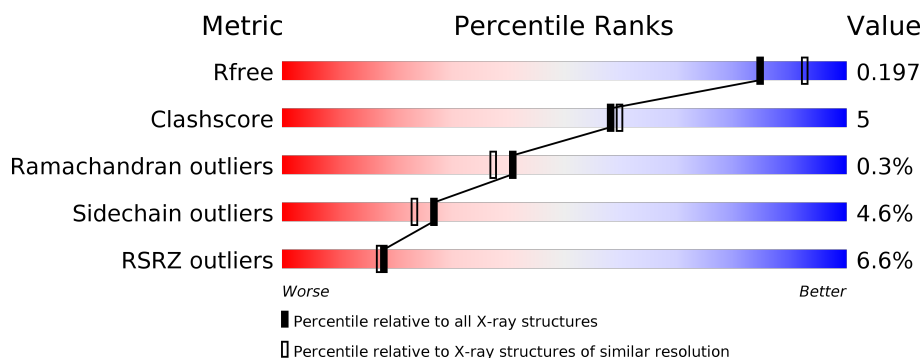
1 Overall quality at a glance ⓘ

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 on 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	325	<div> <div>9%</div> <div>84%</div> <div>11%</div> <div>• •</div> </div>
1	C	325	<div> <div>13%</div> <div>85%</div> <div>10%</div> <div>• •</div> </div>
1	E	325	<div> <div>3%</div> <div>89%</div> <div>8%</div> <div>•</div> </div>
1	G	325	<div> <div>2%</div> <div>89%</div> <div>7%</div> <div>• •</div> </div>
1	I	325	<div> <div>6%</div> <div>87%</div> <div>7%</div> <div>• •</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12729 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 C111S/D83S-C111S HETERODIMER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	7	0
			2267	1384	415	462	6			
1	C	311	Total	C	N	O	S	0	2	0
			2252	1375	413	458	6			
1	E	313	Total	C	N	O	S	0	6	0
			2273	1386	417	464	6			
1	G	313	Total	C	N	O	S	0	7	0
			2273	1386	416	465	6			
1	I	313	Total	C	N	O	S	0	6	0
			2272	1386	415	465	6			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	SER	ASP	microheterogeneity	UNP P00441
A	111	SER	CYS	engineered mutation	UNP P00441
A	154	GLY	-	linker	UNP P00441
A	155	ALA	-	linker	UNP P00441
A	156	ALA	-	linker	UNP P00441
A	157	ALA	-	linker	UNP P00441
A	158	SER	-	linker	UNP P00441
A	159	GLY	-	linker	UNP P00441
A	160	GLY	-	linker	UNP P00441
A	161	GLY	-	linker	UNP P00441
A	162	GLY	-	linker	UNP P00441
A	163	GLY	-	linker	UNP P00441
A	164	SER	-	linker	UNP P00441
A	165	GLY	-	linker	UNP P00441
A	166	GLY	-	linker	UNP P00441
A	167	GLY	-	linker	UNP P00441
A	168	GLY	-	linker	UNP P00441
A	169	SER	-	linker	UNP P00441
A	252	SER	ASP	microheterogeneity	UNP P00441

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Chain	Residue	Modelled	Actual	Comment	Reference
A	280	SER	CYS	engineered mutation	UNP P00441
C	83	SER	ASP	microheterogeneity	UNP P00441
C	111	SER	CYS	engineered mutation	UNP P00441
C	154	GLY	-	linker	UNP P00441
C	155	ALA	-	linker	UNP P00441
C	156	ALA	-	linker	UNP P00441
C	157	ALA	-	linker	UNP P00441
C	158	SER	-	linker	UNP P00441
C	159	GLY	-	linker	UNP P00441
C	160	GLY	-	linker	UNP P00441
C	161	GLY	-	linker	UNP P00441
C	162	GLY	-	linker	UNP P00441
C	163	GLY	-	linker	UNP P00441
C	164	SER	-	linker	UNP P00441
C	165	GLY	-	linker	UNP P00441
C	166	GLY	-	linker	UNP P00441
C	167	GLY	-	linker	UNP P00441
C	168	GLY	-	linker	UNP P00441
C	169	SER	-	linker	UNP P00441
C	252	SER	ASP	microheterogeneity	UNP P00441
C	280	SER	CYS	engineered mutation	UNP P00441
E	83	SER	ASP	microheterogeneity	UNP P00441
E	111	SER	CYS	engineered mutation	UNP P00441
E	154	GLY	-	linker	UNP P00441
E	155	ALA	-	linker	UNP P00441
E	156	ALA	-	linker	UNP P00441
E	157	ALA	-	linker	UNP P00441
E	158	SER	-	linker	UNP P00441
E	159	GLY	-	linker	UNP P00441
E	160	GLY	-	linker	UNP P00441
E	161	GLY	-	linker	UNP P00441
E	162	GLY	-	linker	UNP P00441
E	163	GLY	-	linker	UNP P00441
E	164	SER	-	linker	UNP P00441
E	165	GLY	-	linker	UNP P00441
E	166	GLY	-	linker	UNP P00441
E	167	GLY	-	linker	UNP P00441
E	168	GLY	-	linker	UNP P00441
E	169	SER	-	linker	UNP P00441
E	252	SER	ASP	microheterogeneity	UNP P00441
E	280	SER	CYS	engineered mutation	UNP P00441
G	83	SER	ASP	microheterogeneity	UNP P00441

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Chain	Residue	Modelled	Actual	Comment	Reference
G	111	SER	CYS	engineered mutation	UNP P00441
G	154	GLY	-	linker	UNP P00441
G	155	ALA	-	linker	UNP P00441
G	156	ALA	-	linker	UNP P00441
G	157	ALA	-	linker	UNP P00441
G	158	SER	-	linker	UNP P00441
G	159	GLY	-	linker	UNP P00441
G	160	GLY	-	linker	UNP P00441
G	161	GLY	-	linker	UNP P00441
G	162	GLY	-	linker	UNP P00441
G	163	GLY	-	linker	UNP P00441
G	164	SER	-	linker	UNP P00441
G	165	GLY	-	linker	UNP P00441
G	166	GLY	-	linker	UNP P00441
G	167	GLY	-	linker	UNP P00441
G	168	GLY	-	linker	UNP P00441
G	169	SER	-	linker	UNP P00441
G	252	SER	ASP	microheterogeneity	UNP P00441
G	280	SER	CYS	engineered mutation	UNP P00441
I	83	SER	ASP	microheterogeneity	UNP P00441
I	111	SER	CYS	engineered mutation	UNP P00441
I	154	GLY	-	linker	UNP P00441
I	155	ALA	-	linker	UNP P00441
I	156	ALA	-	linker	UNP P00441
I	157	ALA	-	linker	UNP P00441
I	158	SER	-	linker	UNP P00441
I	159	GLY	-	linker	UNP P00441
I	160	GLY	-	linker	UNP P00441
I	161	GLY	-	linker	UNP P00441
I	162	GLY	-	linker	UNP P00441
I	163	GLY	-	linker	UNP P00441
I	164	SER	-	linker	UNP P00441
I	165	GLY	-	linker	UNP P00441
I	166	GLY	-	linker	UNP P00441
I	167	GLY	-	linker	UNP P00441
I	168	GLY	-	linker	UNP P00441
I	169	SER	-	linker	UNP P00441
I	252	SER	ASP	microheterogeneity	UNP P00441
I	280	SER	CYS	engineered mutation	UNP P00441

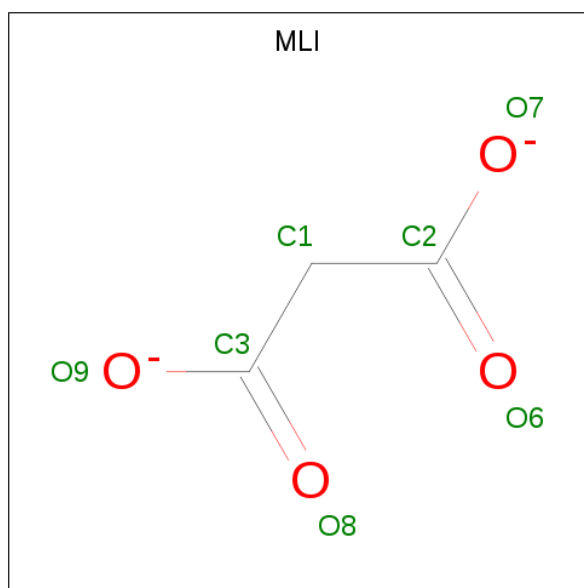
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Zn 2 2	0	0
2	I	2	Total Zn 2 2	0	0
2	A	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	2	Total Cu 4 4	0	2
3	I	2	Total Cu 4 4	0	2
3	A	2	Total Cu 4 4	0	2
3	C	2	Total Cu 3 3	0	1
3	E	2	Total Cu 4 4	0	2

- Molecule 4 is MALONATE ION (three-letter code: MLI) (formula: C₃H₂O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			7	3	4		

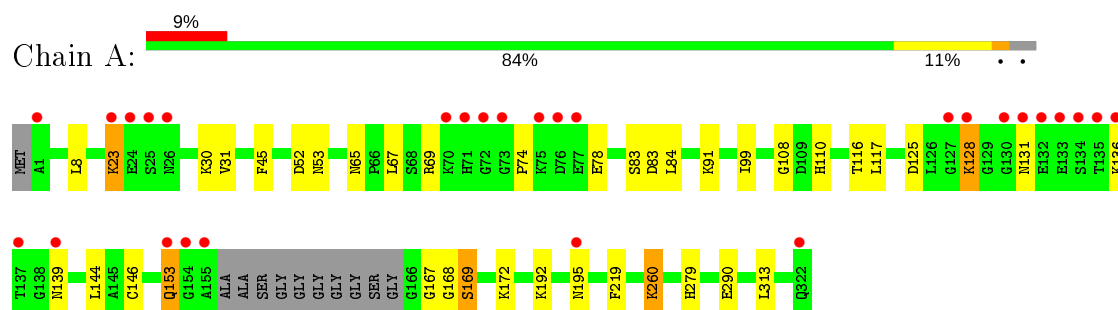
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	226	Total	O	0	0
			226	226		
5	C	141	Total	O	0	0
			141	141		
5	E	368	Total	O	0	0
			368	368		
5	G	324	Total	O	0	0
			324	324		
5	I	297	Total	O	0	0
			297	297		

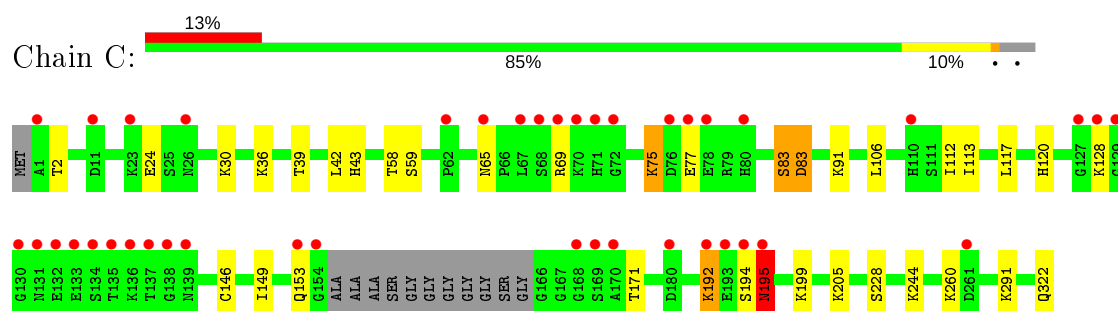
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

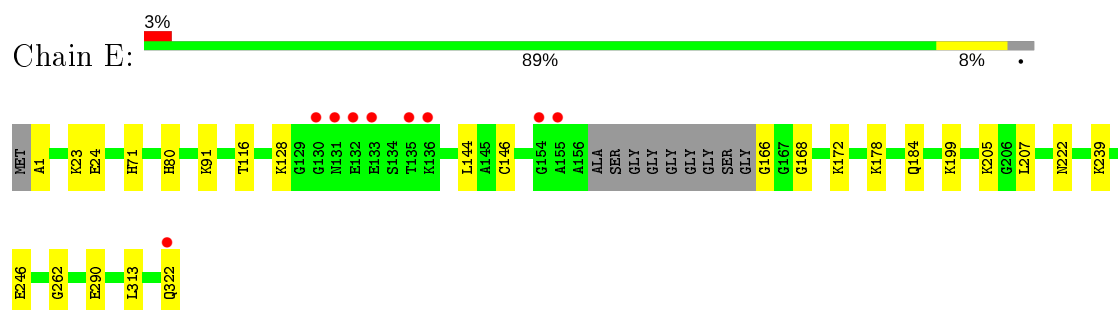
- Molecule 1: Superoxide dismutase C111S/D83S-C111S HETERODIMER



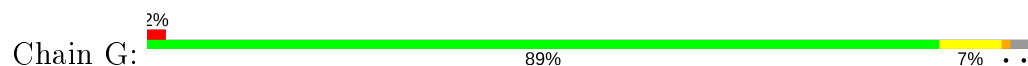
- Molecule 1: Superoxide dismutase C111S/D83S-C111S HETERODIMER

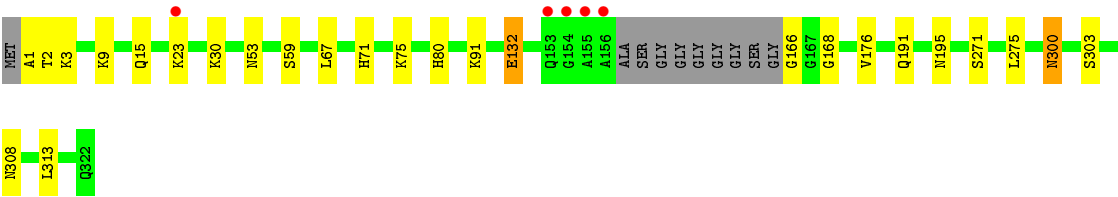


- Molecule 1: Superoxide dismutase C111S/D83S-C111S HETERODIMER

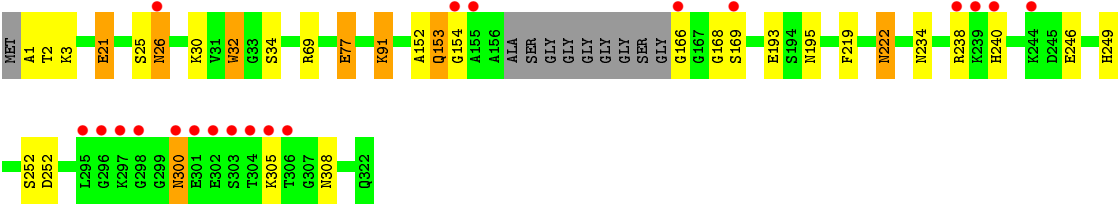
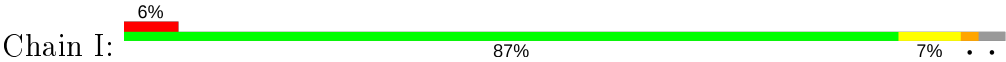


- Molecule 1: Superoxide dismutase C111S/D83S-C111S HETERODIMER





● Molecule 1: Superoxide dismutase C111S/D83S-C111S HETERODIMER



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	162.70Å 201.67Å 143.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.57 – 2.00 47.52 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.57-2.00) 99.9 (47.52-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.156 , 0.190 0.167 , 0.197	Depositor DCC
R_{free} test set	7971 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 61.1	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	0.97	EDS
Total number of atoms	12729	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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: ZN, MLI, 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	0.51	0/2328	0.66	0/3136
1	C	0.49	1/2286 (0.0%)	0.66	1/3078 (0.0%)
1	E	0.56	0/2328	0.71	0/3135
1	G	0.56	0/2333	0.79	4/3142 (0.1%)
1	I	0.54	0/2327	0.71	2/3133 (0.1%)
All	All	0.53	1/11602 (0.0%)	0.71	7/15624 (0.0%)

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	C	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	83[A]	SER	C-O	-6.96	1.10	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	132[A]	GLU	CA-CB-CG	-8.35	95.04	113.40
1	G	132[B]	GLU	CA-CB-CG	-8.35	95.04	113.40
1	G	271[A]	SER	CA-CB-OG	-6.48	93.69	111.20
1	G	271[B]	SER	CA-CB-OG	-6.48	93.69	111.20
1	I	21[A]	GLU	CA-CB-CG	-5.74	100.78	113.40
1	I	21[B]	GLU	CA-CB-CG	-5.74	100.78	113.40
1	C	83[A]	SER	CA-C-O	5.50	131.66	120.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	195	ASN	Peptide
1	C	83[A]	SER	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	2267	0	2188	24	0
1	C	2252	0	2171	13	0
1	E	2273	0	2190	16	0
1	G	2273	0	2191	20	0
1	I	2272	0	2189	32	0
2	A	2	0	0	0	0
2	C	2	0	0	0	0
2	E	2	0	0	0	0
2	G	2	0	0	0	0
2	I	2	0	0	0	0
3	A	4	0	0	0	0
3	C	3	0	0	0	0
3	E	4	0	0	0	0
3	G	4	0	0	0	0
3	I	4	0	0	0	0
4	E	7	0	2	0	0
5	A	226	0	0	10	0
5	C	141	0	0	1	0
5	E	368	0	0	7	0
5	G	324	0	0	9	1
5	I	297	0	0	10	1
All	All	12729	0	10931	102	1

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.

All (102) 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:G:300:ASN:HD21	1:G:308:ASN:HD21	1.26	0.83
1:A:279:HIS:ND1	5:A:502:HOH:O	2.14	0.79
1:A:110:HIS:ND1	5:A:503:HOH:O	2.15	0.79
1:C:39:THR:O	1:C:43:HIS:HE1	1.69	0.75
1:I:300:ASN:HD21	1:I:308:ASN:HD21	1.31	0.75
1:I:222:ASN:ND2	5:I:502:HOH:O	2.20	0.74
1:C:30:LYS:NZ	5:C:501:HOH:O	2.20	0.74
1:G:191:GLN:HE22	1:G:275:LEU:H	1.34	0.74
1:E:222[B]:ASN:ND2	5:E:502:HOH:O	2.19	0.72
1:A:167:GLY:HA3	5:A:585:HOH:O	1.90	0.70
1:G:132[B]:GLU:CD	5:G:502:HOH:O	2.31	0.68
1:G:9:LYS:HD3	5:G:678:HOH:O	1.93	0.67
1:G:168:GLY:HA2	5:G:548:HOH:O	1.95	0.67
1:I:21[B]:GLU:HG2	1:I:32:TRP:HZ3	1.59	0.67
1:G:191:GLN:NE2	1:G:275:LEU:H	1.94	0.66
1:I:168:GLY:HA2	5:I:608:HOH:O	1.96	0.65
1:I:21[B]:GLU:HG3	1:I:30:LYS:HB2	1.77	0.65
1:E:322:GLN:O	5:E:501:HOH:O	2.15	0.64
1:I:91:LYS:HD3	5:I:627:HOH:O	1.99	0.61
1:G:67:LEU:HD23	1:I:26:ASN:HB2	1.84	0.60
1:E:178:LYS:CE	1:E:184:GLN:HE21	2.15	0.60
1:C:192:LYS:HA	1:C:192:LYS:CE	2.32	0.59
1:I:1:ALA:H1	1:I:166:GLY:C	2.06	0.59
1:G:3:LYS:HG2	5:G:731:HOH:O	2.03	0.59
1:I:21[B]:GLU:CD	1:I:32:TRP:CZ3	2.76	0.59
1:C:65:ASN:HD21	1:C:69:ARG:H	1.51	0.59
1:A:168:GLY:HA3	5:A:610:HOH:O	2.03	0.59
1:G:132[B]:GLU:OE1	5:G:502:HOH:O	2.17	0.58
1:I:25:SER:O	1:I:26:ASN:CB	2.49	0.57
1:I:153:GLN:HA	1:I:219:PHE:CE1	2.40	0.56
1:E:168:GLY:HA2	5:E:611:HOH:O	2.06	0.56
1:I:1:ALA:N	1:I:166:GLY:C	2.60	0.55
1:I:21[B]:GLU:CG	1:I:32:TRP:HZ3	2.20	0.54
1:E:166:GLY:N	5:E:511:HOH:O	2.41	0.54
1:G:15:GLN:NE2	5:G:506:HOH:O	2.40	0.52
1:E:199:LYS:NZ	5:E:503:HOH:O	2.24	0.52
1:G:53[B]:ASN:OD1	1:G:176:VAL:HG21	2.10	0.52
1:G:1:ALA:N	1:G:166:GLY:O	2.35	0.51
1:I:152:ALA:O	1:I:154:GLY:N	2.43	0.51
1:A:67:LEU:HB2	1:A:69:ARG:HG3	1.93	0.51
1:G:300:ASN:ND2	1:G:303:SER:H	2.09	0.51
1:I:1:ALA:N	1:I:166:GLY:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:195:ASN:HA	1:I:195:ASN:HA	1.93	0.50
1:G:75:LYS:HD2	5:G:567:HOH:O	2.11	0.50
1:A:23:LYS:CE	1:A:23:LYS:HA	2.43	0.48
1:I:153:GLN:HB3	5:I:525:HOH:O	2.13	0.48
1:E:178:LYS:HE3	1:E:184:GLN:HE21	1.76	0.48
1:I:252[A]:SER:HB3	5:I:556:HOH:O	2.13	0.48
1:C:192:LYS:HA	1:C:192:LYS:HE3	1.96	0.47
1:A:131:ASN:HD21	1:A:139:ASN:HD21	1.62	0.47
1:E:207:LEU:O	1:E:262:GLY:HA2	2.14	0.47
1:A:169:SER:N	5:A:507:HOH:O	2.39	0.47
1:I:234:ASN:HD21	1:I:238:ARG:H	1.62	0.47
1:A:168:GLY:CA	5:A:610:HOH:O	2.63	0.47
1:I:69:ARG:CZ	5:I:639:HOH:O	2.63	0.47
1:I:25:SER:O	1:I:26:ASN:CG	2.53	0.46
1:C:42:LEU:HD13	1:I:153:GLN:HE22	1.81	0.46
1:A:52:ASP:C	1:A:53[B]:ASN:HD22	2.19	0.46
1:I:3:LYS:HG2	1:I:21[A]:GLU:HG3	1.98	0.45
1:C:112:ILE:HD12	1:C:149:ILE:HD13	1.97	0.45
1:C:194:SER:O	1:C:195:ASN:C	2.54	0.45
1:G:71:HIS:HB2	1:G:80:HIS:CE1	2.52	0.45
1:I:77:GLU:CD	1:I:77:GLU:H	2.19	0.45
1:A:108:GLY:HA3	5:A:513:HOH:O	2.15	0.45
1:C:24:GLU:OE1	1:C:24:GLU:N	2.50	0.45
1:I:166:GLY:N	5:I:509:HOH:O	2.49	0.44
1:G:30:LYS:NZ	5:G:514:HOH:O	2.50	0.44
1:C:117:LEU:O	1:C:146:CYS:HA	2.18	0.44
1:E:290:GLU:HA	1:E:313:LEU:HD11	2.00	0.43
1:I:240:HIS:HB2	1:I:249:HIS:CE1	2.53	0.43
1:A:195:ASN:ND2	5:A:517:HOH:O	2.51	0.43
1:I:26:ASN:ND2	1:I:26:ASN:C	2.72	0.43
1:C:43:HIS:HD2	1:C:120:HIS:O	2.02	0.43
1:A:8[B]:LEU:HD11	1:A:117:LEU:HD23	2.01	0.43
1:E:199:LYS:CE	5:E:503:HOH:O	2.63	0.43
1:C:106:LEU:O	1:C:113:ILE:HD12	2.19	0.43
1:A:290:GLU:HA	1:A:313:LEU:HD11	2.01	0.43
1:I:25:SER:O	1:I:26:ASN:OD1	2.37	0.43
1:A:260:LYS:HG3	5:A:620:HOH:O	2.19	0.42
1:I:69:ARG:NE	5:I:516:HOH:O	2.52	0.42
1:A:8[A]:LEU:HD11	1:A:117:LEU:HD23	2.02	0.42
1:E:116:THR:CG2	1:E:146:CYS:HB2	2.49	0.42
1:A:65:ASN:HD21	1:A:69:ARG:H	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:GLN:HA	1:A:219:PHE:CE1	2.55	0.42
1:E:222[B]:ASN:ND2	5:E:522:HOH:O	2.52	0.42
1:G:166:GLY:N	5:G:518:HOH:O	2.53	0.42
1:A:31:VAL:HB	1:A:99:ILE:HB	2.03	0.41
1:I:21[B]:GLU:CD	1:I:32:TRP:HZ3	2.21	0.41
1:E:71:HIS:HB2	1:E:80:HIS:CE1	2.55	0.41
1:E:1:ALA:N	1:E:166:GLY:O	2.31	0.41
1:A:128:LYS:CD	5:A:628:HOH:O	2.68	0.41
1:A:125:ASP:O	1:A:128:LYS:HG3	2.21	0.41
1:A:45:PHE:O	1:A:84:LEU:HB2	2.21	0.41
1:C:75:LYS:HB2	5:I:721:HOH:O	2.20	0.41
1:I:169:SER:HB2	5:I:595:HOH:O	2.21	0.41
1:A:116:THR:CG2	1:A:146:CYS:HB2	2.50	0.41
1:I:25:SER:O	1:I:26:ASN:HB3	2.21	0.40
1:E:178:LYS:HE3	1:E:184:GLN:NE2	2.36	0.40

All (1) 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)
5:G:657:HOH:O	5:I:712:HOH:O[3_455]	2.14	0.06

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	311/325 (96%)	303 (97%)	6 (2%)	2 (1%)	25	19
1	C	305/325 (94%)	290 (95%)	13 (4%)	2 (1%)	22	16
1	E	311/325 (96%)	308 (99%)	3 (1%)	0	100	100
1	G	312/325 (96%)	308 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	311/325 (96%)	303 (97%)	7 (2%)	1 (0%)	41	37
All	All	1550/1625 (95%)	1512 (98%)	33 (2%)	5 (0%)	41	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	153	GLN
1	C	195	ASN
1	I	153	GLN
1	A	153	GLN
1	A	74	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	244/242 (101%)	232 (95%)	12 (5%)	25	21
1	C	239/242 (99%)	222 (93%)	17 (7%)	14	10
1	E	243/242 (100%)	234 (96%)	9 (4%)	34	32
1	G	244/242 (101%)	238 (98%)	6 (2%)	47	49
1	I	243/242 (100%)	231 (95%)	12 (5%)	25	21
All	All	1213/1210 (100%)	1157 (95%)	56 (5%)	27	23

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	30	LYS
1	A	78	GLU
1	A	83[A]	SER
1	A	91	LYS
1	A	128	LYS
1	A	136	LYS

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Mol	Chain	Res	Type
1	A	144	LEU
1	A	169	SER
1	A	172	LYS
1	A	192	LYS
1	A	260	LYS
1	C	2	THR
1	C	36	LYS
1	C	58	THR
1	C	59	SER
1	C	75	LYS
1	C	77	GLU
1	C	91	LYS
1	C	128	LYS
1	C	171	THR
1	C	192	LYS
1	C	199	LYS
1	C	205	LYS
1	C	228	SER
1	C	244	LYS
1	C	260	LYS
1	C	291	LYS
1	C	322	GLN
1	E	23	LYS
1	E	24	GLU
1	E	91	LYS
1	E	128	LYS
1	E	144	LEU
1	E	172	LYS
1	E	205	LYS
1	E	239	LYS
1	E	246	GLU
1	G	2	THR
1	G	23	LYS
1	G	59	SER
1	G	91	LYS
1	G	300	ASN
1	G	313	LEU
1	I	2[A]	THR
1	I	2[B]	THR
1	I	26	ASN
1	I	32	TRP
1	I	34	SER

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Mol	Chain	Res	Type
1	I	77	GLU
1	I	91	LYS
1	I	193	GLU
1	I	222	ASN
1	I	246	GLU
1	I	300	ASN
1	I	305	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	139	ASN
1	C	43	HIS
1	C	65	ASN
1	C	110	HIS
1	C	322	GLN
1	E	184	GLN
1	G	15	GLN
1	G	184	GLN
1	G	191	GLN
1	G	300	ASN
1	I	26	ASN
1	I	153	GLN
1	I	234	ASN
1	I	300	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 29 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	MLI	E	405	-	0,6,6	0.00	-	0,7,7	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MLI	E	405	-	-	0/0/4/4	-

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	314/325 (96%)	0.16	28 (8%) 9 8	24, 36, 86, 105	4 (1%)
1	C	313/325 (96%)	0.62	41 (13%) 3 3	29, 47, 83, 103	4 (1%)
1	E	315/325 (96%)	-0.20	9 (2%) 51 50	18, 27, 57, 83	4 (1%)
1	G	315/325 (96%)	-0.21	5 (1%) 72 70	19, 28, 51, 74	4 (1%)
1	I	315/325 (96%)	-0.04	20 (6%) 20 19	19, 31, 71, 102	4 (1%)
All	All	1572/1625 (96%)	0.06	103 (6%) 18 17	18, 34, 74, 105	20 (1%)

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	70	LYS	6.1
1	A	75	LYS	5.3
1	C	77	GLU	5.1
1	C	26	ASN	5.1
1	C	154	GLY	5.1
1	C	132	GLU	5.0
1	C	67	LEU	4.8
1	I	301	GLU	4.7
1	A	132	GLU	4.7
1	C	169	SER	4.7
1	C	68	SER	4.5
1	A	127	GLY	4.5
1	A	131	ASN	4.4
1	A	23	LYS	4.3
1	A	135	THR	4.2
1	C	137	THR	4.1
1	A	154	GLY	4.1
1	A	71	HIS	4.1
1	C	135	THR	4.1
1	C	195	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	136	LYS	4.0
1	C	110	HIS	3.9
1	C	131	ASN	3.8
1	A	77	GLU	3.7
1	I	297	LYS	3.7
1	A	70	LYS	3.7
1	C	11	ASP	3.6
1	A	137	THR	3.6
1	C	130	GLY	3.6
1	G	155	ALA	3.6
1	A	136	LYS	3.5
1	G	154	GLY	3.5
1	C	69	ARG	3.5
1	I	300	ASN	3.5
1	C	129	GLY	3.5
1	C	192	LYS	3.3
1	I	296	GLY	3.3
1	C	127	GLY	3.3
1	I	298	GLY	3.3
1	A	76	ASP	3.3
1	E	154	GLY	3.2
1	A	25	SER	3.2
1	A	155	ALA	3.2
1	A	24	GLU	3.2
1	E	132	GLU	3.1
1	C	170	ALA	3.1
1	A	130	GLY	3.1
1	C	180	ASP	3.1
1	I	239	LYS	3.0
1	G	153	GLN	3.0
1	C	194	SER	3.0
1	E	131	ASN	3.0
1	A	72	GLY	3.0
1	E	130	GLY	3.0
1	E	133	GLU	3.0
1	C	153	GLN	3.0
1	I	166	GLY	2.9
1	A	133	GLU	2.9
1	C	193	GLU	2.9
1	C	133	GLU	2.9
1	I	302	GLU	2.8
1	C	128	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	78	GLU	2.7
1	I	304	THR	2.7
1	C	139	ASN	2.7
1	C	138	GLY	2.7
1	I	154	GLY	2.6
1	A	153	GLN	2.6
1	I	238	ARG	2.6
1	C	62	PRO	2.6
1	C	80	HIS	2.5
1	A	26	ASN	2.5
1	C	168	GLY	2.5
1	I	169	SER	2.5
1	A	128	LYS	2.5
1	I	306	THR	2.4
1	G	156	ALA	2.4
1	I	303	SER	2.4
1	C	72	GLY	2.4
1	C	134	SER	2.4
1	C	76	ASP	2.4
1	I	305	LYS	2.4
1	C	65	ASN	2.4
1	I	240	HIS	2.4
1	E	135	THR	2.4
1	C	71	HIS	2.3
1	A	195	ASN	2.3
1	A	73	GLY	2.3
1	A	1	ALA	2.3
1	A	322	GLN	2.3
1	G	23	LYS	2.3
1	A	134	SER	2.2
1	A	139	ASN	2.2
1	E	155	ALA	2.1
1	E	322	GLN	2.1
1	I	26	ASN	2.1
1	I	295	LEU	2.1
1	C	23	LYS	2.1
1	E	136	LYS	2.1
1	I	244	LYS	2.1
1	C	261	ASP	2.0
1	I	155	ALA	2.0
1	C	1	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
4	MLI	E	405	7/7	0.89	0.17	49,50,52,54	7
2	ZN	C	401	1/1	0.96	0.07	54,54,54,54	1
3	CU	C	402	1/1	0.96	0.06	49,49,49,49	1
2	ZN	C	403	1/1	0.98	0.06	33,33,33,33	1
2	ZN	A	401	1/1	0.98	0.09	49,49,49,49	1
2	ZN	G	403	1/1	0.99	0.05	34,34,34,34	1
3	CU	A	402[B]	1/1	0.99	0.10	39,39,39,39	1
3	CU	A	402[A]	1/1	0.99	0.10	37,37,37,37	1
3	CU	C	404[B]	1/1	0.99	0.08	30,30,30,30	1
3	CU	I	404[B]	1/1	0.99	0.10	33,33,33,33	1
3	CU	C	404[A]	1/1	0.99	0.08	32,32,32,32	1
3	CU	A	404[A]	1/1	0.99	0.12	31,31,31,31	1
3	CU	G	402[B]	1/1	0.99	0.11	21,21,21,21	1
3	CU	A	404[B]	1/1	0.99	0.12	31,31,31,31	1
3	CU	G	402[A]	1/1	0.99	0.11	23,23,23,23	1
2	ZN	I	403	1/1	0.99	0.05	43,43,43,43	1
3	CU	G	404[B]	1/1	0.99	0.12	28,28,28,28	1
3	CU	G	404[A]	1/1	0.99	0.12	27,27,27,27	1
3	CU	I	404[A]	1/1	0.99	0.10	35,35,35,35	1
2	ZN	A	403	1/1	0.99	0.08	30,30,30,30	1
3	CU	E	404[A]	1/1	1.00	0.08	23,23,23,23	1
3	CU	E	404[B]	1/1	1.00	0.08	21,21,21,21	1
2	ZN	E	403	1/1	1.00	0.06	25,25,25,25	1
3	CU	E	402[A]	1/1	1.00	0.09	28,28,28,28	1
2	ZN	I	401	1/1	1.00	0.09	23,23,23,23	1
3	CU	I	402[B]	1/1	1.00	0.09	23,23,23,23	1
3	CU	I	402[A]	1/1	1.00	0.09	24,24,24,24	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	E	401	1/1	1.00	0.07	29,29,29,29	1
3	CU	E	402[B]	1/1	1.00	0.09	25,25,25,25	1
2	ZN	G	401	1/1	1.00	0.09	26,26,26,26	1

6.5 Other polymers [i](#)

There are no such residues in this entry.