



wwPDB X-ray Structure Validation Summary Report

Mar 1, 2026 – 12:46 AM UTC

PDB ID : 1FBX / pdb_00001fbx
Title : CRYSTAL STRUCTURE OF ZINC-CONTAINING E.COLI GTP CYCLO-HYDROLASE I
Authors : Auerbach, G.; Herrmann, A.; Bracher, A.; Bader, A.; Gutlich, M.; Fischer, M.; Neukamm, M.; Nar, H.; Garrido-Franco, M.; Richardson, J.; Huber, R.; Bacher, A.
Deposited on : 2000-07-17
Resolution : 2.80 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
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

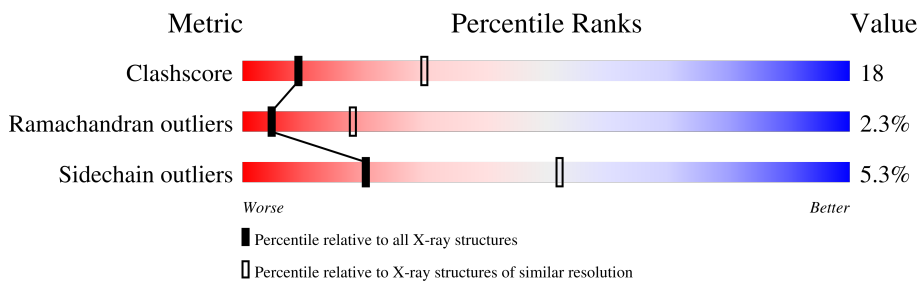
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	221	61% 34% .
1	B	221	65% 33% .
1	C	221	68% 29% .
1	D	221	66% 29% 5%
1	E	221	57% 38% 5%
1	F	221	62% 32% 5%
1	G	221	65% 32% .
1	H	221	62% 33% .

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Mol	Chain	Length	Quality of chain		
1	I	221	57%	38%	5%
1	J	221	58%	37%	5%
1	K	221	60%	36%	5%
1	L	221	58%	37%	5%
1	M	221	57%	36%	7%
1	N	221	55%	40%	•
1	O	221	55%	37%	8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	3350	-	-	X	-
3	CL	F	3355	-	-	X	-
3	CL	J	3354	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26025 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 GTP CYCLOHYDROLASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	221	Total 1732	C 1088	N 309	O 326	S 9	74	0	0
1	B	221	Total 1732	C 1088	N 309	O 326	S 9	74	0	0
1	C	221	Total 1732	C 1088	N 309	O 326	S 9	74	0	0
1	D	221	Total 1732	C 1088	N 309	O 326	S 9	74	0	0
1	E	221	Total 1732	C 1088	N 309	O 326	S 9	74	0	0
1	F	221	Total 1732	C 1088	N 309	O 326	S 9	74	0	0
1	G	221	Total 1732	C 1088	N 309	O 326	S 9	74	0	0
1	H	221	Total 1732	C 1088	N 309	O 326	S 9	74	0	0
1	I	221	Total 1732	C 1088	N 309	O 326	S 9	74	0	0
1	J	221	Total 1732	C 1088	N 309	O 326	S 9	74	0	0
1	K	221	Total 1732	C 1088	N 309	O 326	S 9	74	0	0
1	L	221	Total 1732	C 1088	N 309	O 326	S 9	74	0	0
1	M	221	Total 1732	C 1088	N 309	O 326	S 9	74	0	0
1	N	221	Total 1732	C 1088	N 309	O 326	S 9	74	0	0
1	O	221	Total 1732	C 1088	N 309	O 326	S 9	74	0	0

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

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

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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total Cl 1 1	0	0
3	G	1	Total Cl 1 1	0	0
3	H	1	Total Cl 1 1	0	0
3	I	1	Total Cl 1 1	0	0
3	J	1	Total Cl 1 1	0	0
3	K	1	Total Cl 1 1	0	0
3	L	1	Total Cl 1 1	0	0
3	M	1	Total Cl 1 1	0	0
3	N	1	Total Cl 1 1	0	0
3	O	1	Total Cl 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 1 1	0	0
4	B	1	Total O 1 1	0	0
4	C	1	Total O 1 1	0	0
4	D	1	Total O 1 1	0	0
4	E	1	Total O 1 1	0	0
4	F	1	Total O 1 1	0	0
4	G	1	Total O 1 1	0	0
4	H	1	Total O 1 1	0	0
4	I	1	Total O 1 1	0	0

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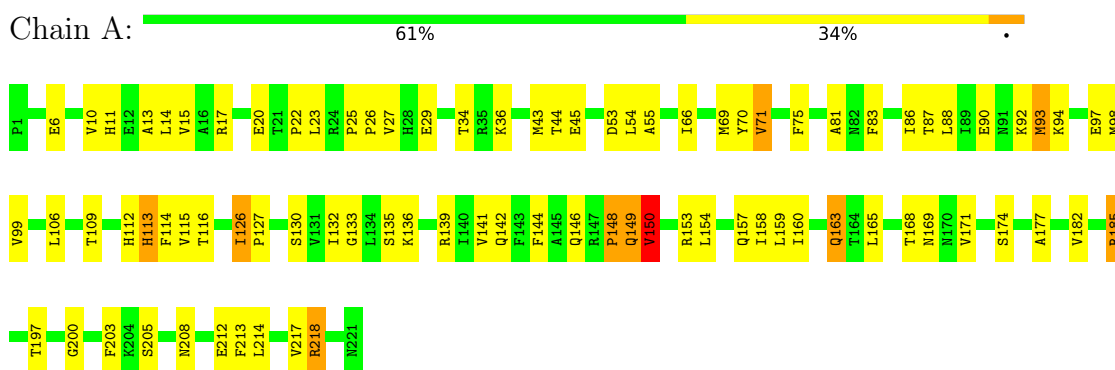
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	J	1	Total O 1 1	0	0
4	K	1	Total O 1 1	0	0
4	L	1	Total O 1 1	0	0
4	M	1	Total O 1 1	0	0
4	N	1	Total O 1 1	0	0
4	O	1	Total O 1 1	0	0

3 Residue-property plots

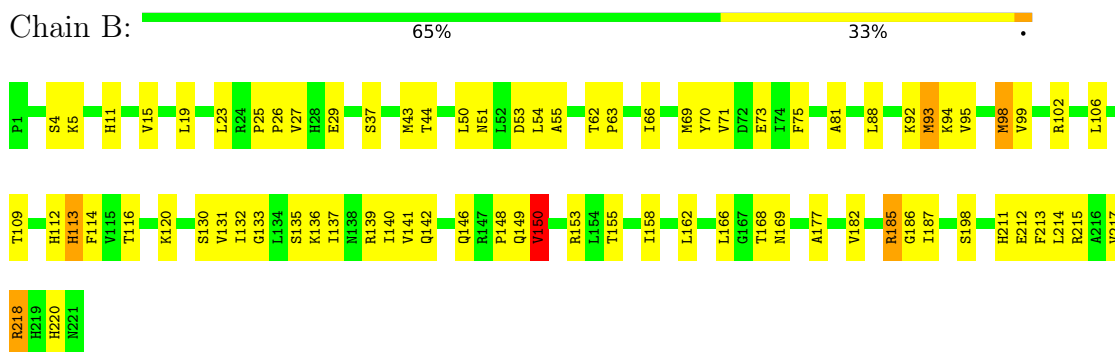
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

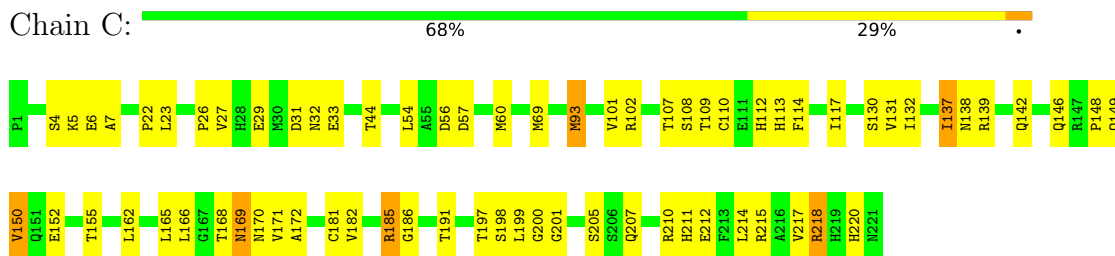
- Molecule 1: GTP CYCLOHYDROLASE I



- Molecule 1: GTP CYCLOHYDROLASE I

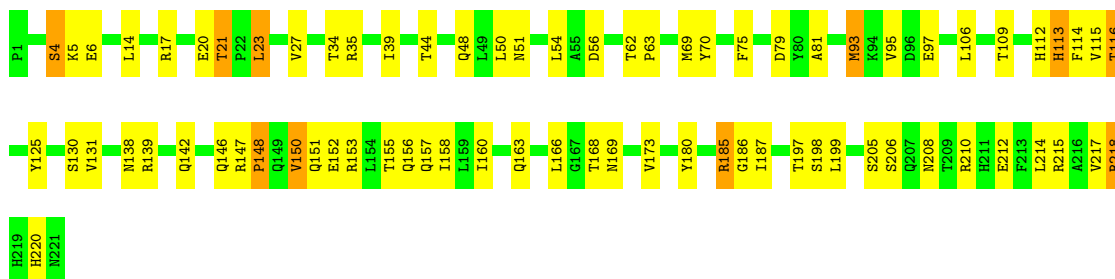


- Molecule 1: GTP CYCLOHYDROLASE I



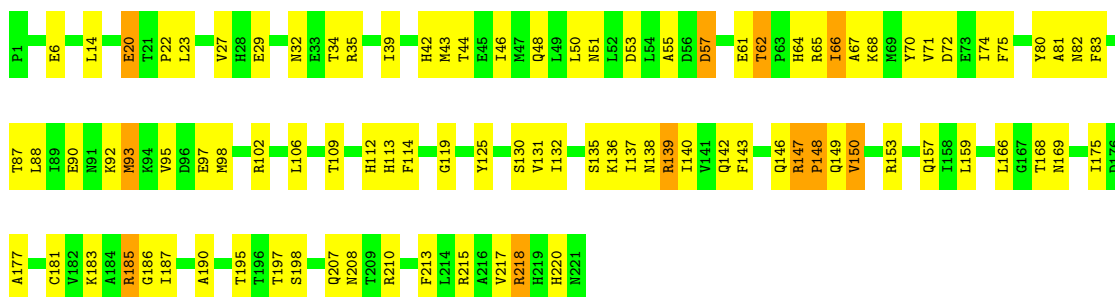
- Molecule 1: GTP CYCLOHYDROLASE I

Chain D:  66% 29% 5%



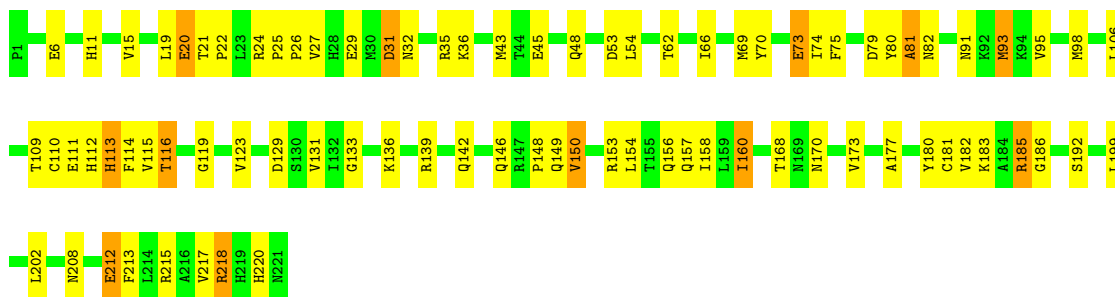
• Molecule 1: GTP CYCLOHYDROLASE I

Chain E:  57% 38% 5%



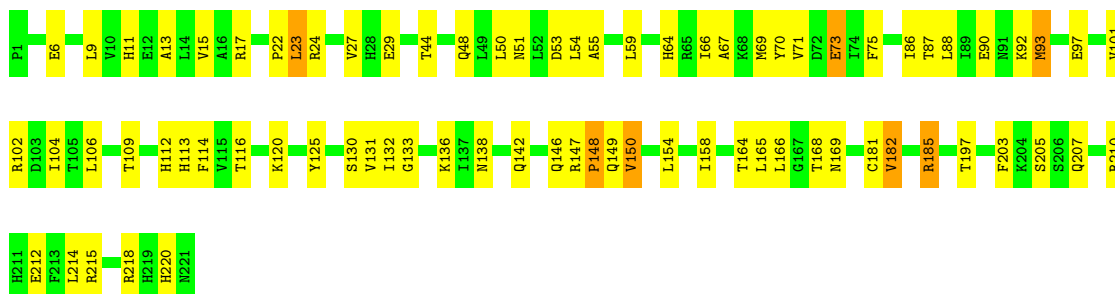
• Molecule 1: GTP CYCLOHYDROLASE I

Chain F:  62% 32% 5%



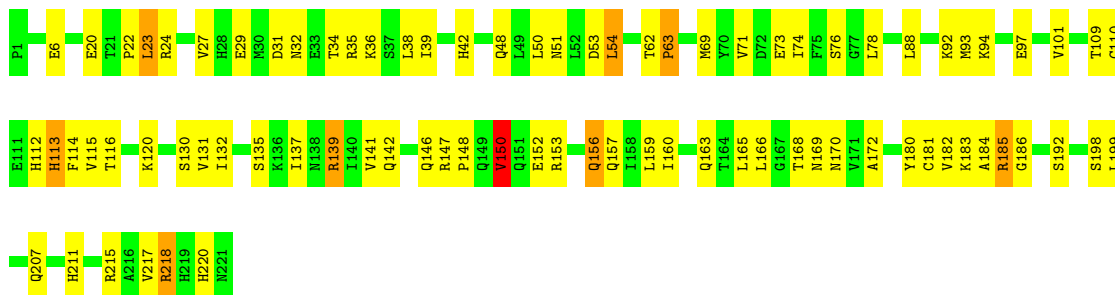
• Molecule 1: GTP CYCLOHYDROLASE I

Chain G:  65% 32% 3%



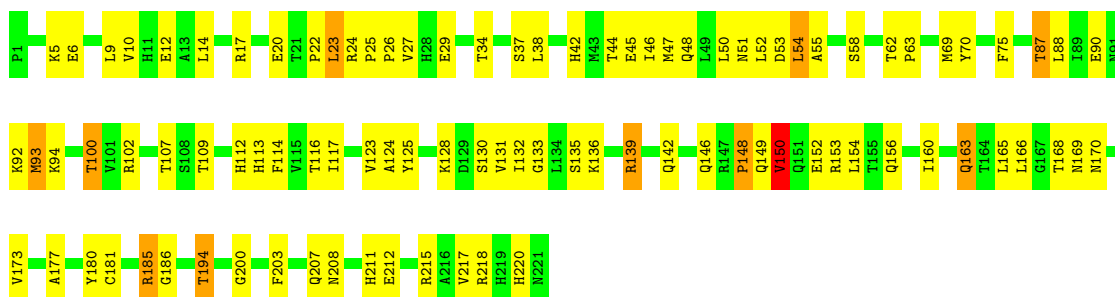
- Molecule 1: GTP CYCLOHYDROLASE I

Chain H:  62% 33%



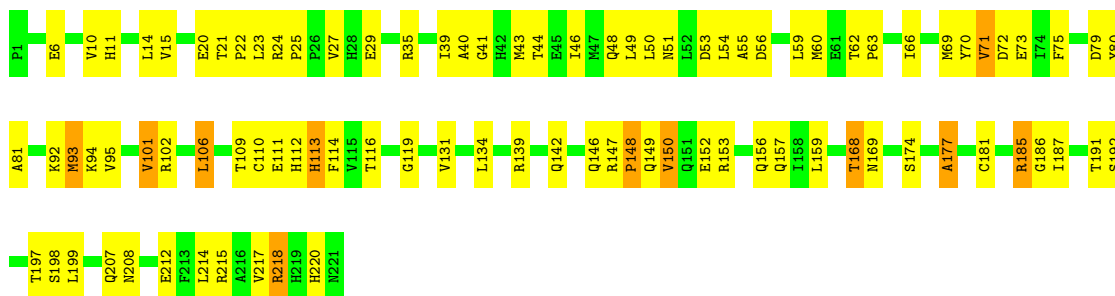
- Molecule 1: GTP CYCLOHYDROLASE I

Chain I:  57% 38% 5%



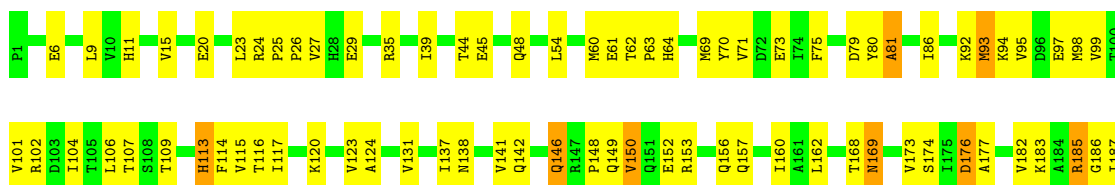
- Molecule 1: GTP CYCLOHYDROLASE I

Chain J:  58% 37% 5%



- Molecule 1: GTP CYCLOHYDROLASE I

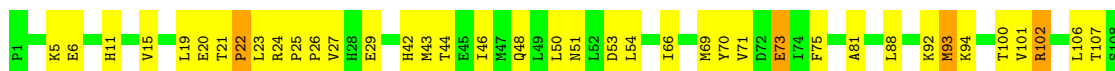
Chain K:  60% 36% 5%





- Molecule 1: GTP CYCLOHYDROLASE I

Chain L: 58% 37% 5%



- Molecule 1: GTP CYCLOHYDROLASE I

Chain M: 57% 36% 7%



- Molecule 1: GTP CYCLOHYDROLASE I

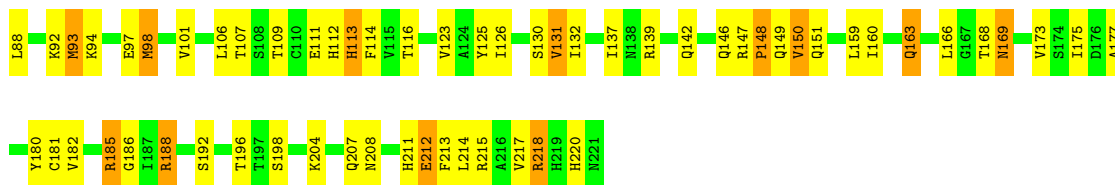
Chain N: 55% 40% .



- Molecule 1: GTP CYCLOHYDROLASE I

Chain O: 55% 37% 8%





4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	227.69Å 314.19Å 132.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.98 – 2.80	Depositor
% Data completeness (in resolution range)	91.2 (14.98-2.80)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.202 , 0.251	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	26025	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

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, CL

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	0.73	1/1760 (0.1%)	1.20	18/2384 (0.8%)
1	B	0.76	1/1760 (0.1%)	1.16	14/2384 (0.6%)
1	C	0.79	1/1760 (0.1%)	1.17	14/2384 (0.6%)
1	D	0.77	1/1760 (0.1%)	1.14	11/2384 (0.5%)
1	E	0.65	0/1760	1.18	13/2384 (0.5%)
1	F	0.69	0/1760	1.13	14/2384 (0.6%)
1	G	0.61	0/1760	1.08	13/2384 (0.5%)
1	H	0.69	0/1760	1.15	12/2384 (0.5%)
1	I	0.62	0/1760	1.05	7/2384 (0.3%)
1	J	0.65	0/1760	1.12	15/2384 (0.6%)
1	K	0.67	0/1760	1.13	12/2384 (0.5%)
1	L	0.59	0/1760	1.04	10/2384 (0.4%)
1	M	0.66	0/1760	1.18	20/2384 (0.8%)
1	N	0.60	0/1760	1.10	10/2384 (0.4%)
1	O	0.61	1/1760 (0.1%)	1.08	14/2384 (0.6%)
All	All	0.68	5/26400 (0.0%)	1.13	197/35760 (0.6%)

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	D	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	MET	SD-CE	-5.89	1.64	1.79
1	C	69	MET	SD-CE	-5.46	1.66	1.79
1	D	69	MET	SD-CE	-5.36	1.66	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	69	MET	SD-CE	-5.35	1.66	1.79
1	O	69	MET	SD-CE	-5.21	1.66	1.79

The worst 5 of 197 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	147	ARG	CA-C-N	-9.41	110.02	119.90
1	M	147	ARG	C-N-CA	-9.41	110.02	119.90
1	O	73	GLU	N-CA-C	9.25	123.75	108.48
1	H	150	VAL	N-CA-C	-9.25	94.80	108.12
1	K	150	VAL	N-CA-C	-9.21	94.86	108.12

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	180	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1732	0	1766	56	0
1	B	1732	0	1766	49	0
1	C	1732	0	1766	42	0
1	D	1732	0	1766	43	0
1	E	1732	0	1766	60	0
1	F	1732	0	1766	76	0
1	G	1732	0	1766	69	0
1	H	1732	0	1766	68	0
1	I	1732	0	1766	88	0
1	J	1732	0	1766	98	0
1	K	1732	0	1766	75	0
1	L	1732	0	1766	79	0
1	M	1732	0	1766	84	0
1	N	1732	0	1766	94	0
1	O	1732	0	1766	107	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
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
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
3	A	1	0	0	2	0
3	B	1	0	0	0	0
3	C	1	0	0	1	0
3	D	1	0	0	1	0
3	E	1	0	0	1	0
3	F	1	0	0	2	0
3	G	1	0	0	1	0
3	H	1	0	0	1	0
3	I	1	0	0	1	0
3	J	1	0	0	2	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	1	0
3	N	1	0	0	1	0
3	O	1	0	0	1	0
4	A	1	0	0	1	0
4	B	1	0	0	2	0
4	C	1	0	0	1	0
4	D	1	0	0	1	0
4	E	1	0	0	1	0
4	F	1	0	0	2	0
4	G	1	0	0	1	0
4	H	1	0	0	2	0
4	I	1	0	0	1	0
4	J	1	0	0	3	0
4	K	1	0	0	0	0
4	L	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	1	0	0	1	0
4	N	1	0	0	1	0
4	O	1	0	0	2	0
All	All	26025	0	26490	919	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 18.

The worst 5 of 919 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:J:69:MET:HE2	1:N:185:ARG:HD2	1.27	1.14
1:C:168:THR:HG22	1:C:170:ASN:H	1.14	1.11
1:I:168:THR:HG22	1:I:170:ASN:H	1.22	1.04
1:F:185:ARG:HD2	1:M:69:MET:HE2	1.39	1.02
1:K:61:GLU:OE1	1:K:64:HIS:HD2	1.41	1.00

There are no symmetry-related clashes.

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	219/221 (99%)	206 (94%)	9 (4%)	4 (2%)	6	23
1	B	219/221 (99%)	204 (93%)	11 (5%)	4 (2%)	6	23
1	C	219/221 (99%)	200 (91%)	13 (6%)	6 (3%)	4	15
1	D	219/221 (99%)	200 (91%)	16 (7%)	3 (1%)	9	30
1	E	219/221 (99%)	199 (91%)	14 (6%)	6 (3%)	4	15
1	F	219/221 (99%)	196 (90%)	17 (8%)	6 (3%)	4	15
1	G	219/221 (99%)	195 (89%)	20 (9%)	4 (2%)	6	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	219/221 (99%)	202 (92%)	11 (5%)	6 (3%)	4	15
1	I	219/221 (99%)	197 (90%)	16 (7%)	6 (3%)	4	15
1	J	219/221 (99%)	196 (90%)	18 (8%)	5 (2%)	5	18
1	K	219/221 (99%)	201 (92%)	14 (6%)	4 (2%)	6	23
1	L	219/221 (99%)	191 (87%)	24 (11%)	4 (2%)	6	23
1	M	219/221 (99%)	199 (91%)	14 (6%)	6 (3%)	4	15
1	N	219/221 (99%)	196 (90%)	16 (7%)	7 (3%)	3	11
1	O	219/221 (99%)	197 (90%)	16 (7%)	6 (3%)	4	15
All	All	3285/3315 (99%)	2979 (91%)	229 (7%)	77 (2%)	5	18

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	VAL
1	A	218	ARG
1	B	27	VAL
1	F	27	VAL
1	K	27	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/194 (100%)	186 (96%)	8 (4%)	27	62
1	B	194/194 (100%)	185 (95%)	9 (5%)	24	58
1	C	194/194 (100%)	183 (94%)	11 (6%)	18	49
1	D	194/194 (100%)	183 (94%)	11 (6%)	18	49
1	E	194/194 (100%)	180 (93%)	14 (7%)	13	39
1	F	194/194 (100%)	189 (97%)	5 (3%)	40	75
1	G	194/194 (100%)	183 (94%)	11 (6%)	18	49
1	H	194/194 (100%)	183 (94%)	11 (6%)	18	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	194/194 (100%)	179 (92%)	15 (8%)	12	36
1	J	194/194 (100%)	187 (96%)	7 (4%)	31	66
1	K	194/194 (100%)	183 (94%)	11 (6%)	18	49
1	L	194/194 (100%)	187 (96%)	7 (4%)	31	66
1	M	194/194 (100%)	180 (93%)	14 (7%)	13	39
1	N	194/194 (100%)	184 (95%)	10 (5%)	21	53
1	O	194/194 (100%)	183 (94%)	11 (6%)	18	49
All	All	2910/2910 (100%)	2755 (95%)	155 (5%)	20	52

5 of 155 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	113	HIS
1	N	208	ASN
1	L	185	ARG
1	M	163	GLN
1	O	113	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	146	GLN
1	M	163	GLN
1	O	112	HIS
1	F	211	HIS
1	F	207	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 30 ligands modelled in this entry, 30 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.