W O R L D W I D E

wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jun 15, 2024 – 08:14 PM EDT

PDB ID	:	1USY
Title	:	ATP phosphoribosyl transferase (HisG:HisZ) complex from Thermotoga maritima
Authors	:	Vega, M.C.; Fernandez, F.J.; Murphy, G.E.; Zou, P.; Popov, A.; Wilmanns, M.
Deposited on	:	2003-12-01
Resolution	:	2.52 Å(reported)

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

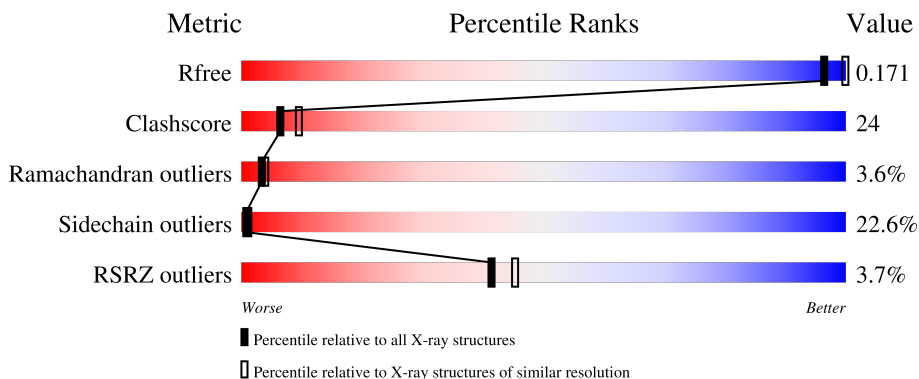|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.52 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	Percentile Ranks	Value
Rfree		0.171
Clashscore		24
Ramachandran outliers		3.6%
Sidechain outliers		22.6%
RSRZ outliers		3.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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 <=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	275	2% / 54% 32% 12% •
1	B	275	4% / 52% 35% 12% •
1	D	275	5% / 45% 42% 12% •
2	C	275	5% / 56% 28% 13% •
3	E	208	5% / 45% 40% 11% •

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Mol	Chain	Length	Quality of chain
3	F	208	2% / 53% / 32% / 11%
3	G	208	5% / 50% / 36% / 12%
4	H	208	% / 48% / 41% / 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
5	HIS	C	1275	-	-	X	-
5	HIS	E	1204	-	-	X	-
5	HIS	E	1205	-	-	X	-
5	HIS	F	1204	-	-	X	X
5	HIS	G	1206	-	-	X	-
5	HIS	H	1203	-	-	X	-
5	HIS	H	1204	-	-	X	-
6	PO4	E	1202	-	-	X	-
6	PO4	H	1202	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 15636 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 ATP PHOSPHORIBOSYLTRANSFERASE REGULATORY SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total 2210	C 1423	N 353	O 429	S 5	14	0	0
1	B	275	Total 2210	C 1423	N 353	O 429	S 5	17	0	0
1	D	274	Total 2202	C 1418	N 352	O 428	S 4	11	0	0

- Molecule 2 is a protein called ATP PHOSPHORIBOSYLTRANSFERASE REGULATORY SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	275	Total 2206	C 1422	N 353	O 427	S 4	23	0	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	68	GLU	ASP	conflict	UNP Q9X0D3
C	134	LEU	VAL	conflict	UNP Q9X0D3

- Molecule 3 is a protein called ATP PHOSPHORIBOSYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	202	Total 1599	C 1027	N 273	O 291	S 8	7	0	1
3	F	203	Total 1605	C 1030	N 274	O 293	S 8	2	0	1
3	G	204	Total 1613	C 1034	N 276	O 295	S 8	0	0	1

- Molecule 4 is a protein called ATP PHOSPHORIBOSYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	202	Total 1599	C 1028	N 274	O 289	S 8	5	0	1

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	186	LYS	GLU	conflict	UNP Q9X0D2

- Molecule 5 is HISTIDINE (three-letter code: HIS) (formula: $C_6H_{10}N_3O_2$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total 11	C 6	N 3	O 2	0	0
5	D	1	Total 11	C 6	N 3	O 2	5	0
5	E	1	Total 11	C 6	N 3	O 2	3	0
5	E	1	Total 11	C 6	N 3	O 2	2	0
5	F	1	Total 11	C 6	N 3	O 2	2	0
5	G	1	Total 11	C 6	N 3	O 2	0	0
5	H	1	Total 11	C 6	N 3	O 2	0	0
5	H	1	Total 11	C 6	N 3	O 2	0	0

• Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
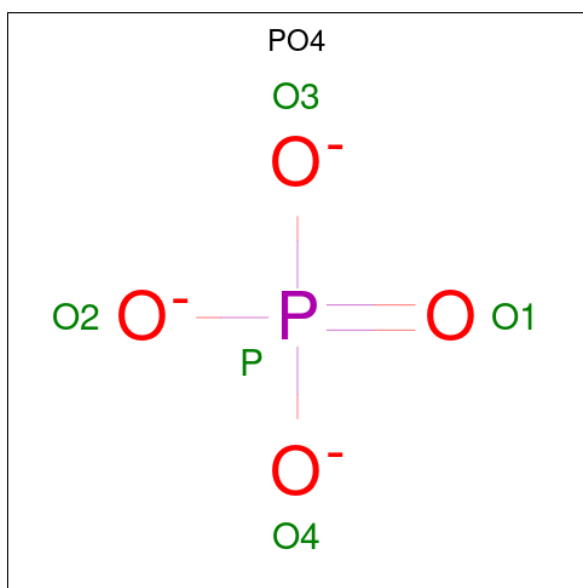
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	O	P	0	0
			5	4	1		
6	E	1	Total	O	P	0	0
			5	4	1		
6	F	1	Total	O	P	0	0
			5	4	1		
6	G	1	Total	O	P	0	0
			5	4	1		
6	G	1	Total	O	P	0	0
			5	4	1		
6	H	1	Total	O	P	0	0
			5	4	1		

• Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	41	Total	O	0	0
			41	41		
7	B	40	Total	O	0	0
			40	40		
7	C	50	Total	O	0	0
			50	50		
7	D	42	Total	O	0	0
			42	42		
7	E	20	Total	O	0	0
			20	20		

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	F	31	Total 31	O 31	0	0
7	G	27	Total 27	O 27	0	0
7	H	23	Total 23	O 23	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 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.
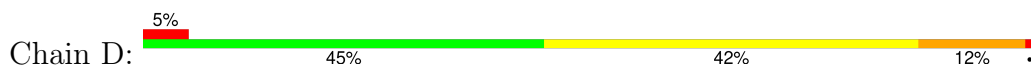
- Molecule 1: ATP PHOSPHORIBOSYLTRANSFERASE REGULATORY SUBUNIT
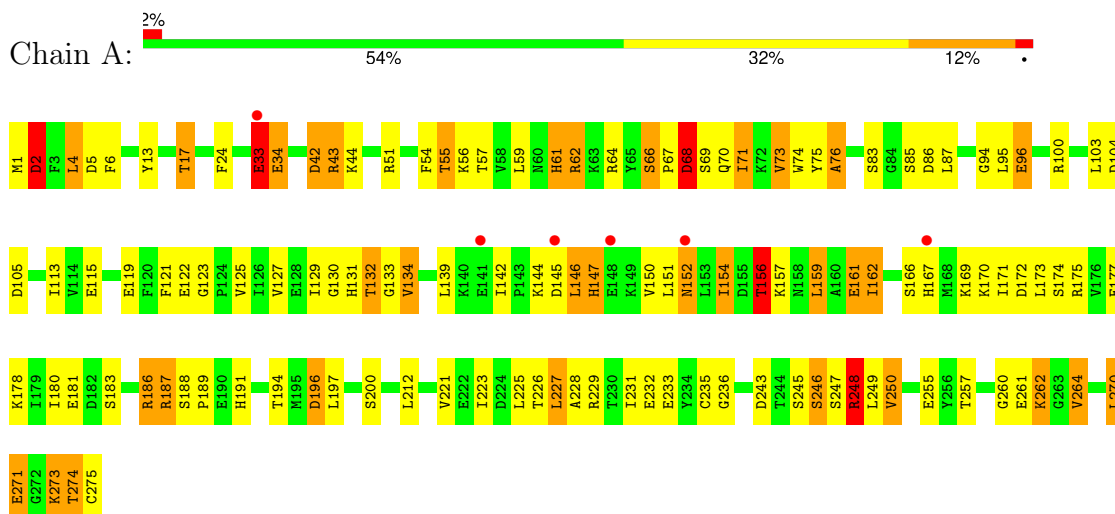
Chain A:

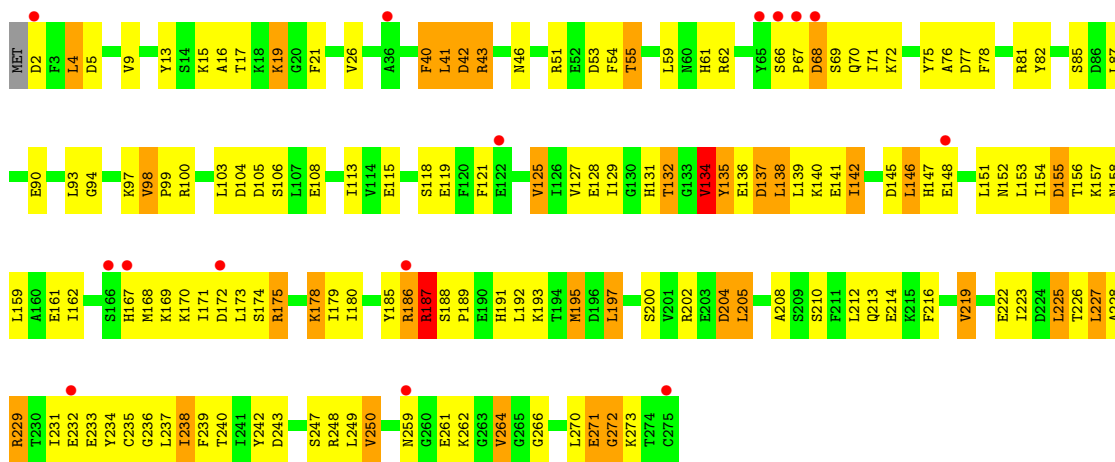
- Molecule 1: ATP PHOSPHORIBOSYLTRANSFERASE REGULATORY SUBUNIT

Chain B:

- Molecule 1: ATP PHOSPHORIBOSYLTRANSFERASE REGULATORY SUBUNIT

Chain D:
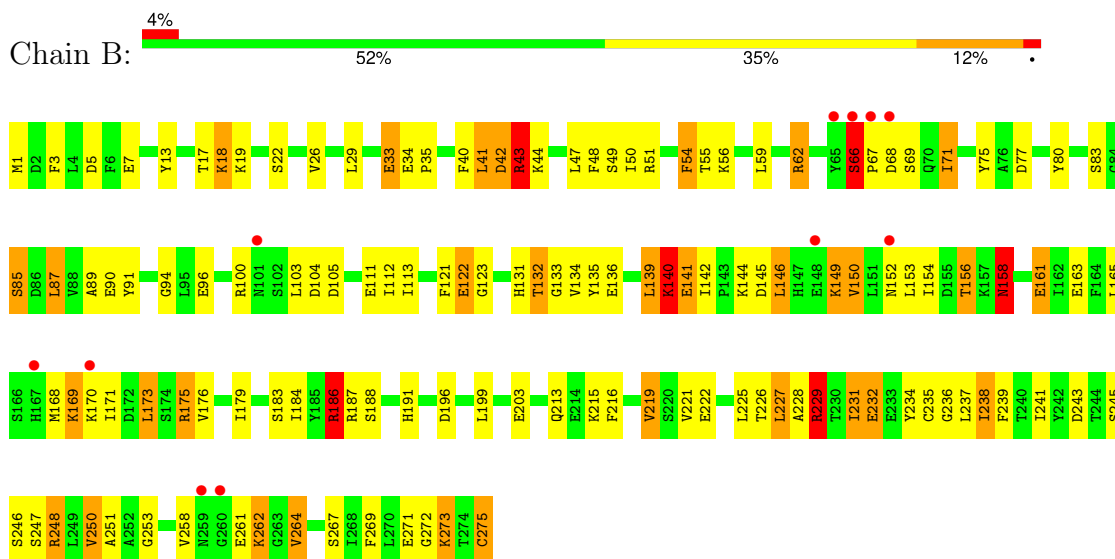
• Molecule 2: ATP PHOSPHORIBOSYLTRANSFERASE REGULATORY SUBUNIT
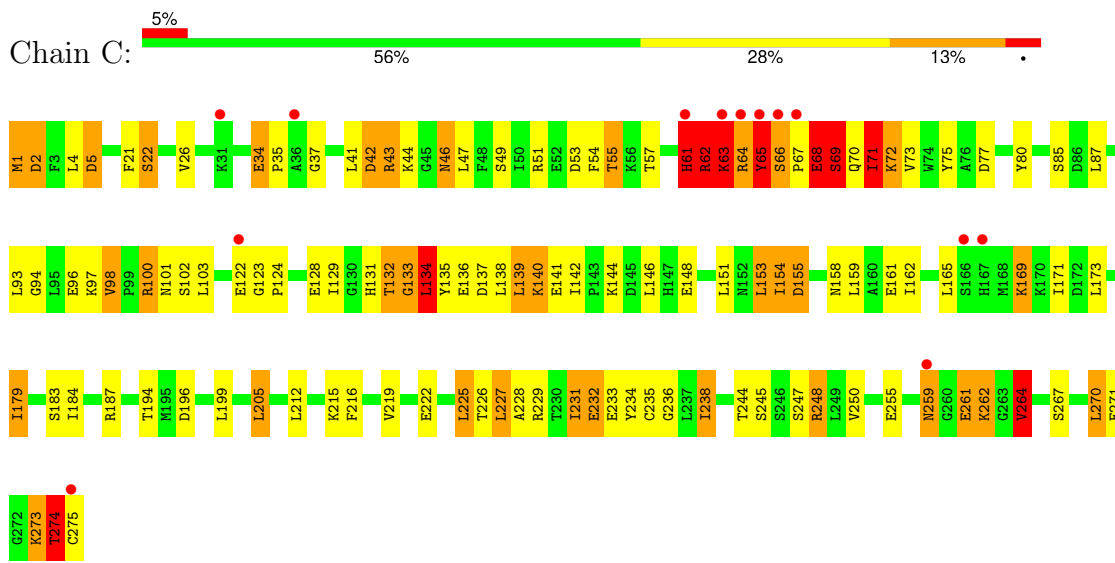
Chain C:

• Molecule 3: ATP PHOSPHORIBOSYLTRANSFERASE

Chain E:

• Molecule 3: ATP PHOSPHORIBOSYLTRANSFERASE

Chain F:

[Chain F sequence diagram with colored residue blocks]

• Molecule 3: ATP PHOSPHORIBOSYLTRANSFERASE

Chain G:
5%
50%   36%   12%

[Chain G sequence diagram with colored residue blocks]
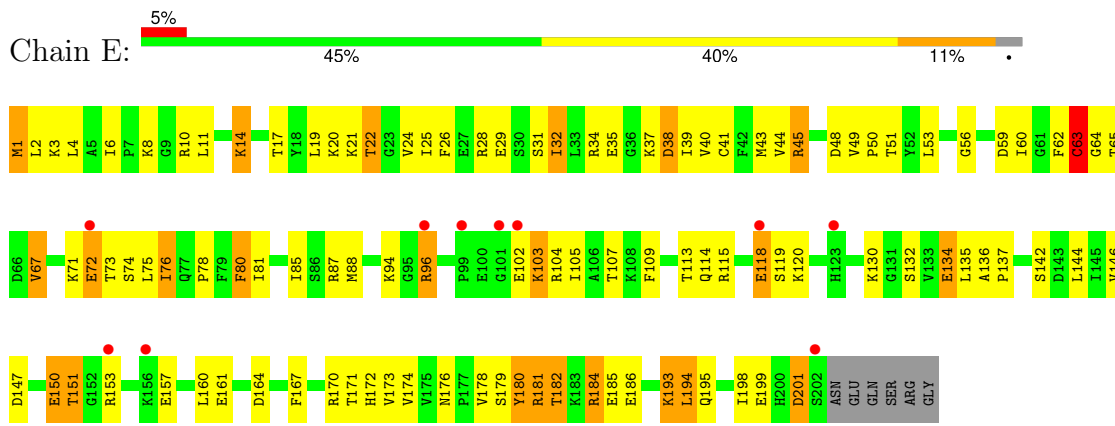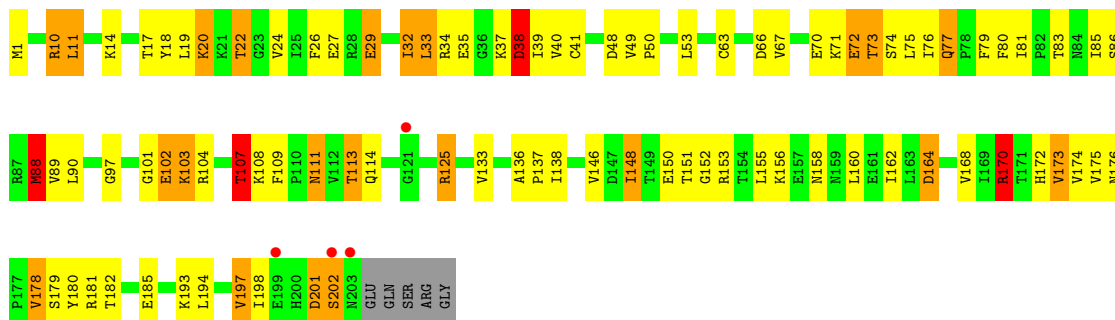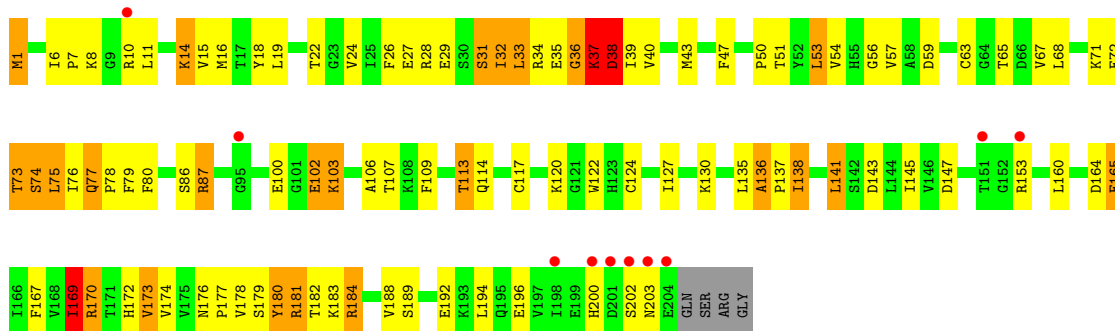
• Molecule 4: ATP PHOSPHORIBOSYLTRANSFERASE

Chain H:
%
48%   41%   8%

[Chain H sequence diagram with colored residue blocks]
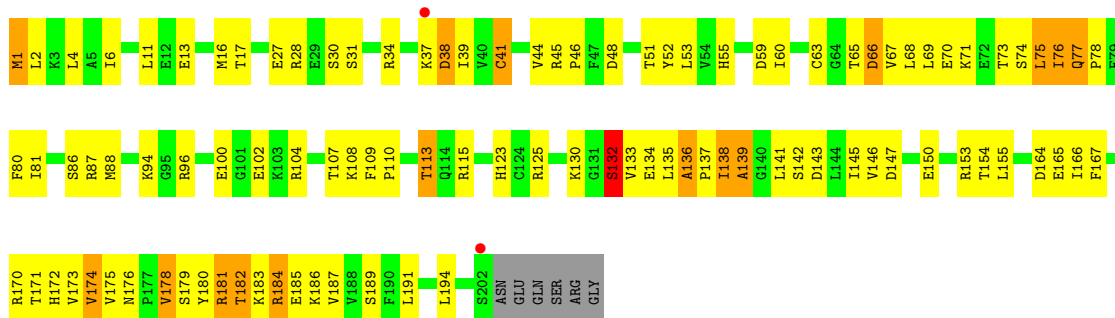
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	101.58Å 134.40Å 154.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.52 12.00 – 2.53	Depositor EDS
% Data completeness (in resolution range)	98.1 (12.00-2.52) 98.4 (12.00-2.53)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	10.70 (at 2.52Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.203 , 0.287 0.209 , 0.171	Depositor DCC
R_{free} test set	518 reflections (0.75%)	wwPDB-VP
Wilson B-factor (Å^2)	50.0	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 59.6	EDS
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15636	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.95% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.93	3/2256 (0.1%)	1.11	16/3043 (0.5%)
1	B	1.34	2/2256 (0.1%)	1.02	12/3043 (0.4%)
1	D	0.78	0/2248	1.01	13/3033 (0.4%)
2	C	0.83	1/2252 (0.0%)	1.08	16/3039 (0.5%)
3	E	0.79	2/1628 (0.1%)	1.01	7/2200 (0.3%)
3	F	1.14	4/1634 (0.2%)	1.09	9/2208 (0.4%)
3	G	0.72	2/1642 (0.1%)	0.97	8/2219 (0.4%)
4	H	0.91	2/1628 (0.1%)	1.01	7/2199 (0.3%)
All	All	0.96	16/15544 (0.1%)	1.04	88/20984 (0.4%)

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	2
1	B	0	1
2	C	0	2
3	F	0	1
All	All	0	6

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	275	CYS	CB-SG	-51.19	0.95	1.82
3	F	125	ARG	NE-CZ	33.64	1.76	1.33
4	H	100	GLU	CD-OE1	19.19	1.46	1.25
1	A	33	GLU	C-N	-17.25	0.94	1.34
1	A	34	GLU	CG-CD	-13.40	1.31	1.51

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	125	ARG	NE-CZ-NH2	-18.39	111.10	120.30
1	A	34	GLU	CG-CD-OE1	-17.38	83.55	118.30
1	A	34	GLU	CG-CD-OE2	13.97	146.24	118.30
3	F	125	ARG	NE-CZ-NH1	13.03	126.81	120.30
4	H	181	ARG	NE-CZ-NH2	-9.39	115.61	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	33	GLU	Mainchain
1	A	34	GLU	Sidechain
1	B	122	GLU	Peptide
2	C	71	ILE	Mainchain
2	C	98	VAL	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	2210	0	2196	90	0
1	B	2210	0	2197	103	0
1	D	2202	0	2185	108	1
2	C	2206	0	2196	106	0
3	E	1599	0	1664	92	0
3	F	1605	0	1669	73	0
3	G	1613	0	1675	90	1
4	H	1599	0	1671	102	0
5	C	11	0	6	7	0
5	D	11	0	6	0	0
5	E	22	0	12	15	0
5	F	11	0	6	8	0
5	G	11	0	6	6	0
5	H	22	0	12	23	0
6	E	10	0	0	2	0
6	F	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	10	0	0	0	0
6	H	5	0	0	2	0
7	A	41	0	0	4	0
7	B	40	0	0	0	0
7	C	50	0	0	5	0
7	D	42	0	0	2	0
7	E	20	0	0	2	0
7	F	31	0	0	1	0
7	G	27	0	0	3	0
7	H	23	0	0	3	0
All	All	15636	0	15501	735	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 24.

The worst 5 of 735 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)
4:H:78:PRO:CB	5:H:1203:HIS:O	1.77	1.30
3:E:65:THR:HG1	5:E:1205:HIS:CE1	1.53	1.26
2:C:72:LYS:O	2:C:73:VAL:HG13	1.42	1.19
5:E:1205:HIS:O	5:E:1205:HIS:CD2	1.94	1.19
5:E:1205:HIS:O	5:E:1205:HIS:HD2	1.24	1.16

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)
1:D:214:GLU:OE1	3:G:1:MET:N[4_554]	2.13	0.07

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	273/275 (99%)	238 (87%)	25 (9%)	10 (4%)	3	4
1	B	273/275 (99%)	242 (89%)	24 (9%)	7 (3%)	5	7
1	D	272/275 (99%)	237 (87%)	25 (9%)	10 (4%)	3	4
2	C	273/275 (99%)	238 (87%)	17 (6%)	18 (7%)	1	1
3	E	200/208 (96%)	183 (92%)	11 (6%)	6 (3%)	4	5
3	F	201/208 (97%)	183 (91%)	11 (6%)	7 (4%)	3	4
3	G	202/208 (97%)	180 (89%)	15 (7%)	7 (4%)	3	4
4	H	200/208 (96%)	190 (95%)	6 (3%)	4 (2%)	7	11
All	All	1894/1932 (98%)	1691 (89%)	134 (7%)	69 (4%)	3	4

5 of 69 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	ALA
1	A	174	SER
1	A	227	LEU
1	A	271	GLU
1	B	141	GLU

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	247/247 (100%)	193 (78%)	54 (22%)	1	1
1	B	247/247 (100%)	190 (77%)	57 (23%)	1	1
1	D	246/247 (100%)	188 (76%)	58 (24%)	1	1
2	C	246/247 (100%)	191 (78%)	55 (22%)	1	1
3	E	181/187 (97%)	136 (75%)	45 (25%)	0	1
3	F	182/187 (97%)	141 (78%)	41 (22%)	1	1
3	G	183/187 (98%)	141 (77%)	42 (23%)	1	1
4	H	181/187 (97%)	145 (80%)	36 (20%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1713/1736 (99%)	1325 (77%)	388 (23%)	1 1

5 of 388 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	25	ILE
3	F	83	THR
3	E	63	CYS
3	E	173	VAL
3	F	155	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
3	E	55	HIS
3	F	84	ASN
3	F	77	GLN
3	F	172	HIS
1	B	131	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

14 ligands are modelled in this entry.

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	#$|Z| > 2$
5	HIS	D	1276	-	6,11,11	1.08	1 (16%)	5,14,14	2.99	3 (60%)
5	HIS	H	1203	-	6,11,11	0.85	0	5,14,14	1.52	1 (20%)
5	HIS	C	1275	-	6,11,11	1.04	1 (16%)	5,14,14	1.64	2 (40%)
5	HIS	H	1204	-	6,11,11	0.96	1 (16%)	5,14,14	1.64	1 (20%)
6	PO4	H	1202	-	4,4,4	1.02	0	6,6,6	0.21	0
6	PO4	F	1203	-	4,4,4	1.15	0	6,6,6	0.72	0
5	HIS	E	1204	-	6,11,11	1.26	1 (16%)	5,14,14	1.71	2 (40%)
5	HIS	E	1205	-	6,11,11	1.24	1 (16%)	5,14,14	2.10	2 (40%)
5	HIS	G	1206	-	6,11,11	1.02	1 (16%)	5,14,14	2.27	2 (40%)
6	PO4	E	1203	-	4,4,4	1.19	0	6,6,6	0.50	0
6	PO4	G	1205	-	4,4,4	0.93	0	6,6,6	0.58	0
6	PO4	E	1202	-	4,4,4	1.30	0	6,6,6	0.98	0
6	PO4	G	1204	-	4,4,4	1.09	0	6,6,6	0.67	0
5	HIS	F	1204	-	6,11,11	1.02	1 (16%)	5,14,14	2.14	2 (40%)

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
5	HIS	D	1276	-	-	6/8/8/8	0/1/1/1
5	HIS	H	1203	-	-	4/8/8/8	0/1/1/1
5	HIS	C	1275	-	-	4/8/8/8	0/1/1/1
5	HIS	H	1204	-	-	4/8/8/8	0/1/1/1
5	HIS	E	1204	-	-	5/8/8/8	0/1/1/1
5	HIS	E	1205	-	-	4/8/8/8	0/1/1/1
5	HIS	G	1206	-	-	5/8/8/8	0/1/1/1
5	HIS	F	1204	-	-	6/8/8/8	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1205	HIS	OXT-C	-2.53	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1276	HIS	OXT-C	-2.38	1.23	1.30
5	C	1275	HIS	OXT-C	-2.29	1.23	1.30
5	E	1204	HIS	CA-N	2.24	1.60	1.48
5	G	1206	HIS	OXT-C	-2.21	1.23	1.30

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	1276	HIS	OXT-C-O	-5.44	111.74	124.08
5	G	1206	HIS	OXT-C-O	-4.02	114.96	124.08
5	F	1204	HIS	OXT-C-O	-3.59	115.94	124.08
5	E	1205	HIS	OXT-C-O	-3.38	116.41	124.08
5	E	1205	HIS	CD2-NE2-CE1	2.53	109.71	105.72

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1275	HIS	CA-CB-CG-ND1
5	C	1275	HIS	CA-CB-CG-CD2
5	D	1276	HIS	O-C-CA-N
5	D	1276	HIS	C-CA-CB-CG
5	E	1204	HIS	O-C-CA-N

There are no ring outliers.

9 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	1203	HIS	12	0
5	C	1275	HIS	7	0
5	H	1204	HIS	11	0
6	H	1202	PO4	2	0
5	E	1204	HIS	9	0
5	E	1205	HIS	6	0
5	G	1206	HIS	6	0
6	E	1202	PO4	2	0
5	F	1204	HIS	8	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	33:GLU	C	34:GLU	N	0.94

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	275/275 (100%)	-0.10	6 (2%)	62	65	9, 27, 50, 61	3 (1%)
1	B	275/275 (100%)	-0.09	11 (4%)	38	42	10, 27, 53, 65	6 (2%)
1	D	274/275 (99%)	-0.04	15 (5%)	25	27	8, 28, 49, 61	4 (1%)
2	C	275/275 (100%)	-0.13	13 (4%)	31	34	11, 26, 54, 78	7 (2%)
3	E	202/208 (97%)	-0.01	10 (4%)	28	31	28, 50, 86, 98	2 (0%)
3	F	203/208 (97%)	-0.08	4 (1%)	65	68	10, 27, 50, 62	1 (0%)
3	G	204/208 (98%)	-0.07	10 (4%)	29	32	11, 27, 48, 60	0
4	H	202/208 (97%)	-0.22	2 (0%)	82	84	9, 27, 46, 58	3 (1%)
All	All	1910/1932 (98%)	-0.09	71 (3%)	41	45	8, 28, 58, 98	26 (1%)

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	202	SER	8.0
2	C	65	TYR	7.6
1	D	68	ASP	6.0
2	C	64	ARG	5.4
3	F	203	ASN	5.3

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 monosaccharides 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
5	HIS	F	1204	11/11	0.71	0.42	40,65,69,72	11
5	HIS	H	1203	11/11	0.73	0.24	63,68,76,78	11
5	HIS	E	1204	11/11	0.80	0.30	40,52,55,59	11
5	HIS	E	1205	11/11	0.80	0.28	40,64,71,72	11
5	HIS	G	1206	11/11	0.82	0.19	70,74,82,87	10
5	HIS	C	1275	11/11	0.88	0.20	57,62,64,66	10
5	HIS	H	1204	11/11	0.88	0.22	67,71,77,77	10
6	PO4	F	1203	5/5	0.89	0.15	61,63,68,69	5
6	PO4	H	1202	5/5	0.89	0.17	71,71,74,74	5
5	HIS	D	1276	11/11	0.90	0.16	40,58,76,78	11
6	PO4	E	1203	5/5	0.92	0.21	63,63,67,69	5
6	PO4	G	1205	5/5	0.93	0.17	41,47,49,53	5
6	PO4	G	1204	5/5	0.96	0.12	63,66,67,68	0
6	PO4	E	1202	5/5	0.97	0.10	43,43,48,54	5

6.5 Other polymers ⓘ

There are no such residues in this entry.