



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:44 AM GMT

PDB ID : 2E2G
Title : Crystal structure of archaeal peroxiredoxin, thioredoxin peroxidase from *Aeropyrum pernix* K1 (pre-oxidation form)
Authors : Nakamura, T.; Yamamoto, T.; Abe, M.; Matsumura, H.; Hagihara, Y.; Goto, T.; Yamaguchi, T.; Inoue, T.
Deposited on : 2006-11-13
Resolution : 2.40 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

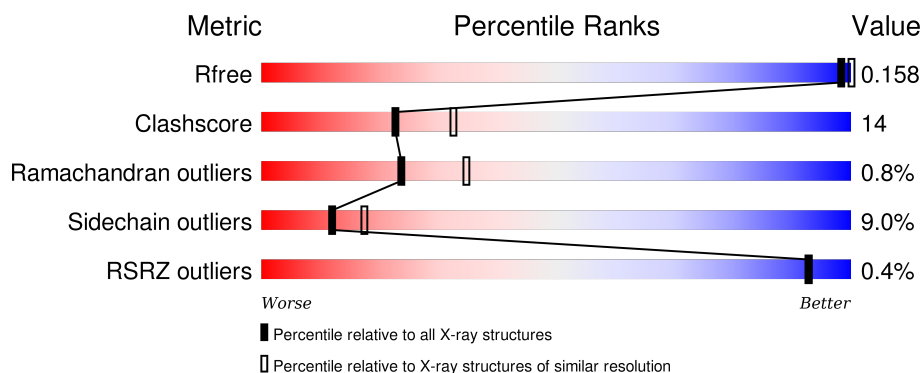
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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. 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	250	<div> <div></div> <div>70% 21% 5%</div> </div>
1	B	250	<div> <div></div> <div>64% 25% 5%</div> </div>
1	C	250	<div> <div></div> <div>64% 26% 5%</div> </div>
1	D	250	<div> <div></div> <div>69% 22% 5%</div> </div>
1	E	250	<div> <div></div> <div>66% 22% 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	250	<div><div></div><div>66%22%5%•5%</div></div>
1	G	250	<div><div></div><div>67%23%••5%</div></div>
1	H	250	<div><div></div><div>66%22%5%•5%</div></div>
1	I	250	<div><div>%</div><div></div><div>63%29%••5%</div></div>
1	J	250	<div><div></div><div>69%22%•5%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19878 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 Probable peroxiredoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	0	0
			1932	1244	339	343	6			
1	B	239	Total	C	N	O	S	0	0	0
			1942	1250	342	344	6			
1	C	239	Total	C	N	O	S	0	0	0
			1938	1247	340	345	6			
1	D	238	Total	C	N	O	S	0	0	0
			1932	1244	339	343	6			
1	E	238	Total	C	N	O	S	0	0	0
			1932	1244	339	343	6			
1	F	238	Total	C	N	O	S	0	0	0
			1932	1244	339	343	6			
1	G	238	Total	C	N	O	S	0	0	0
			1932	1244	339	343	6			
1	H	238	Total	C	N	O	S	0	0	0
			1932	1244	339	343	6			
1	I	238	Total	C	N	O	S	0	0	0
			1932	1244	339	343	6			
1	J	238	Total	C	N	O	S	0	0	0
			1932	1244	339	343	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	207	SER	CYS	ENGINEERED	UNP Q9Y9L0
B	207	SER	CYS	ENGINEERED	UNP Q9Y9L0
C	207	SER	CYS	ENGINEERED	UNP Q9Y9L0
D	207	SER	CYS	ENGINEERED	UNP Q9Y9L0
E	207	SER	CYS	ENGINEERED	UNP Q9Y9L0
F	207	SER	CYS	ENGINEERED	UNP Q9Y9L0
G	207	SER	CYS	ENGINEERED	UNP Q9Y9L0
H	207	SER	CYS	ENGINEERED	UNP Q9Y9L0
I	207	SER	CYS	ENGINEERED	UNP Q9Y9L0

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Chain	Residue	Modelled	Actual	Comment	Reference
J	207	SER	CYS	ENGINEERED	UNP Q9Y9L0

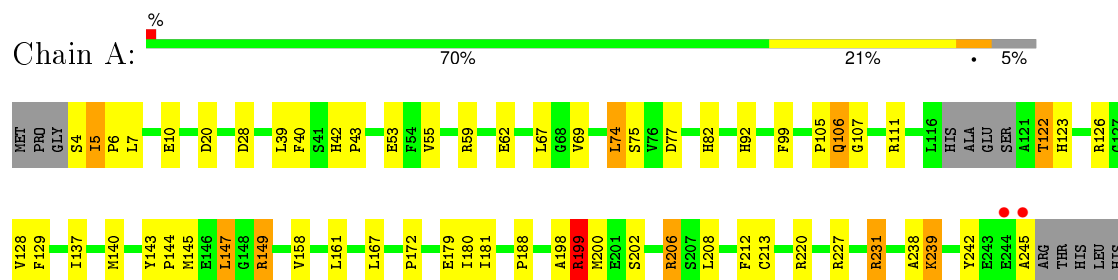
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	57	Total O 57 57	0	0
2	B	60	Total O 60 60	0	0
2	C	39	Total O 39 39	0	0
2	D	57	Total O 57 57	0	0
2	E	65	Total O 65 65	0	0
2	F	59	Total O 59 59	0	0
2	G	61	Total O 61 61	0	0
2	H	65	Total O 65 65	0	0
2	I	30	Total O 30 30	0	0
2	J	49	Total O 49 49	0	0

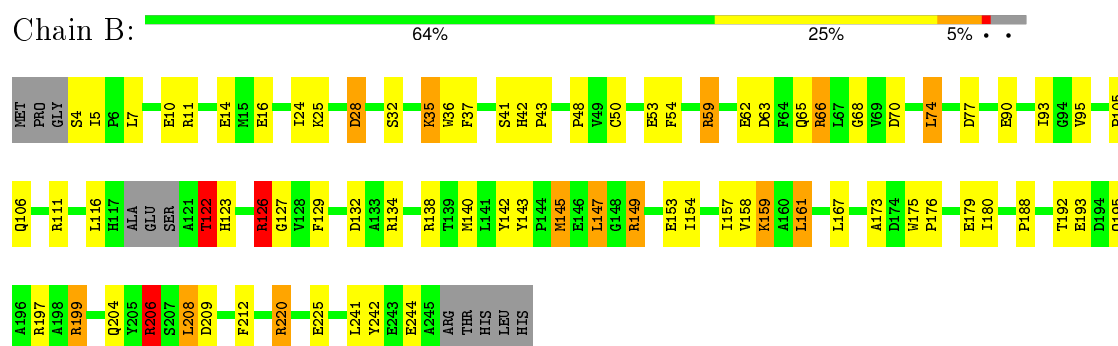
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

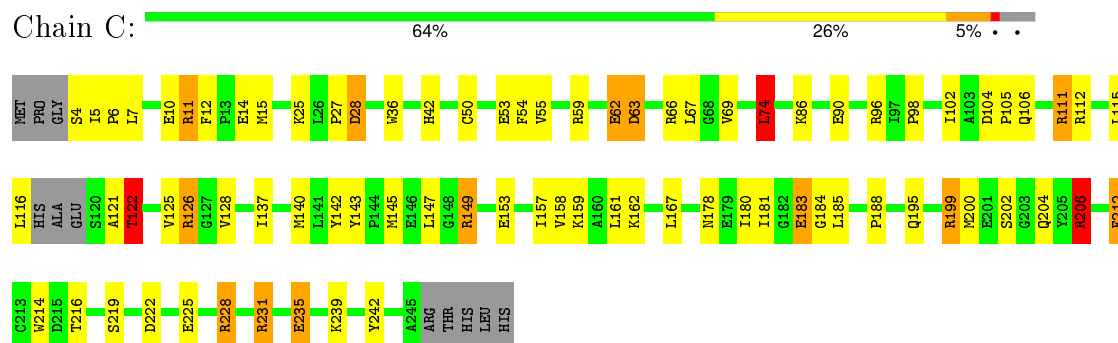
- Molecule 1: Probable peroxiredoxin



- Molecule 1: Probable peroxiredoxin

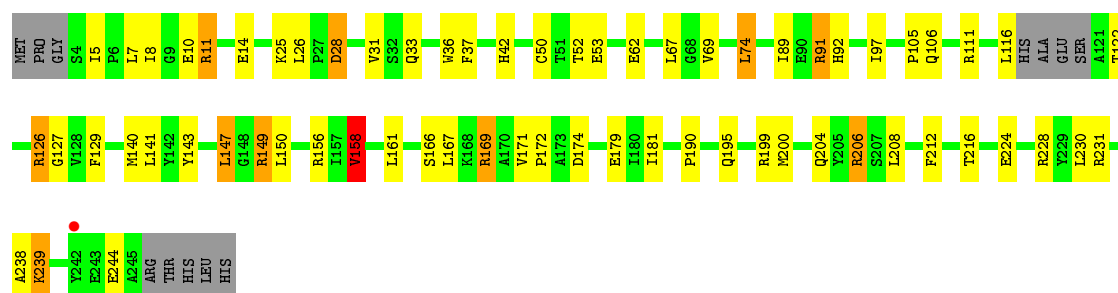


- Molecule 1: Probable peroxiredoxin

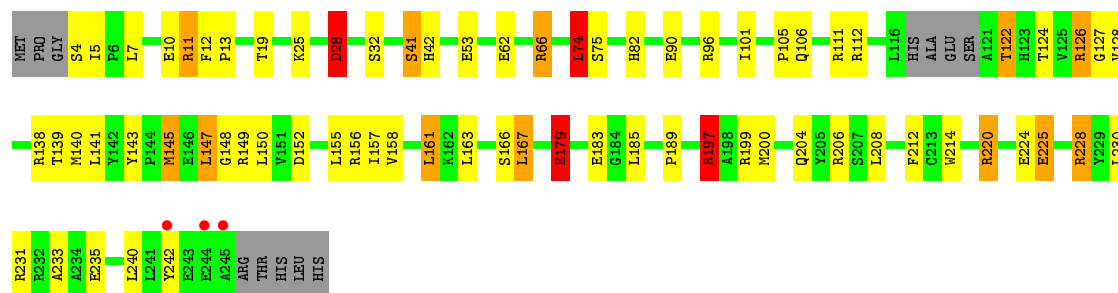


- Molecule 1: Probable peroxiredoxin

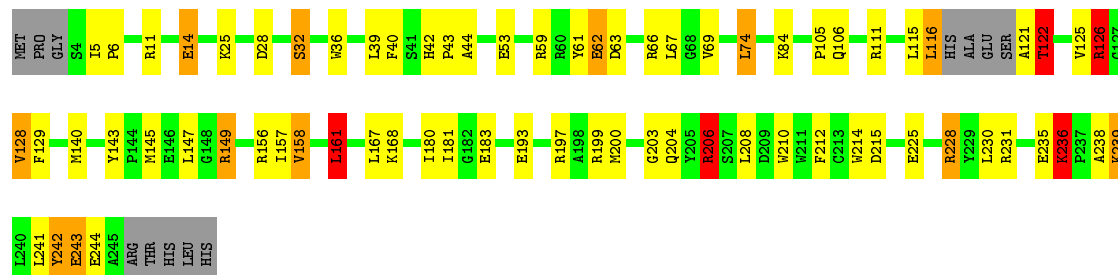




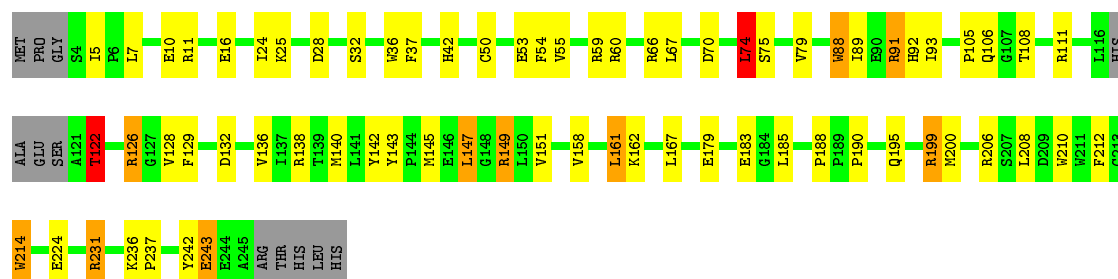
- Molecule 1: Probable peroxiredoxin



- Molecule 1: Probable peroxiredoxin



- Molecule 1: Probable peroxiredoxin



- Molecule 1: Probable peroxiredoxin

E226	E225	ALA	GLU	GLY	MET
A226	A226	ALA	GLU	GLY	P90
R228	R228	A121	A121	S4	T5
Y229	Y229	T122	T122	R11	E14
R231	R231	V125	V125	R126	K25
E235	E235	G127	G127	V128	D28
K239	K239	F129	F129	D132	F37
Y242	Y242	R138	R138	T139	V38
A245	A245	M140	M140	Y143	L39
ARG	ARG	P143	P143	E146	H42
THR	THR	M145	M145	V49	P48
HIS	HIS	L147	L147	G148	C50
LEU	LEU	R149	R149	R156	T51
HIS	HIS	I157	I157	K159	T52
		V158	V158	A160	E53
		L161	L161	L167	F54
				E179	V55
		E183	E183	P188	R59
				E193	E62
		D194	D194	R197	Q65
		A198	A198	R199	V69
		M200	M200	E201	D70
				S207	L74
		L208	L208	D209	V79
		M210	M210	E211	T83
		F212	F212	M214	K84
		C213	C213	Y222	H85
					K86
					R91
					F99
					P100
					I101
					P105
					Q106
					R111
					L116
					H16

- Chain I:  63% 29% 5%

F212	C213	W214	E220	E224	R228	K236	P237	K239	Y242	E243	E244	A245	ARG	THR	HIS	LEU	HIS	HIS	ALA	GLU	SER	A121	T122	R126	G127	V128	F129	T139	L141	Y142	Y143	P144	M145	E146	L147	G148	R149	R156	I157	V158	L161	L167	K168	R169	A170	V171	W175	P176	N177	H178	E179	I180	I181	L185	L186	V187	P188	Q195	R199	M200	R206	S207	L208	D209	W210	S211	F212	C213	W214	E220	E224	R228	K236	P237	K239	Y242	E243	E244	A245	ARG	THR	HIS	LEU	HIS	HIS	ALA	GLU	SER	A121	T122	R126	G127	V128	F129	T139	L141	Y142	Y143	P144	M145	E146	L147	G148	R149	R156	I157	V158	L161	L167	K168	R169	A170	V171	W175	P176	N177	H178	E179	I180	I181	L185	L186	V187	P188	Q195	R199	M200	R206	S207	L208	D209	W210	S211	F212	C213	W214	E220	E224	R228	K236	P237	K239	Y242	E243	E244	A245	ARG	THR	HIS	LEU	HIS	HIS	ALA	GLU	SER	A121	T122	R126	G127	V128	F129	T139	L141	Y142	Y143	P144	M145	E146	L147	G148	R149	R156	I157	V158	L161	L167	K168	R169	A170	V171	W175	P176	N177	H178	E179	I180	I181	L185	L186	V187	P188	Q195	R199	M200	R206	S207	L208	D209	W210	S211	F212	C213	W214	E220	E224	R228	K236	P237	K239	Y242	E243	E244	A245	ARG	THR	HIS	LEU	HIS	HIS	ALA	GLU	SER	A121	T122	R126	G127	V128	F129	T139	L141	Y142	Y143	P144	M145	E146	L147	G148	R149	R156	I157	V158	L161	L167	K168	R169	A170	V171	W175	P176	N177	H178	E179	I180	I181	L185	L186	V187	P188	Q195	R199	M200	R206	S207	L208	D209	W210	S211	F212	C213	W214	E220	E224	R228	K236	P237	K239	Y242	E243	E244	A245	ARG	THR	HIS	LEU	HIS	HIS	ALA	GLU	SER	A121	T122	R126	G127	V128	F129	T139	L141	Y142	Y143	P144	M145	E146	L147	G148	R149	R156	I157	V158	L161	L167	K168	R169	A170	V171	W175	P176	N177	H178	E179	I180	I181	L185	L186	V187	P188	Q195	R199	M200	R206	S207	L208	D209	W210	S211	F212	C213	W214	E220	E224	R228	K236	P237	K239	Y242	E243	E244	A245	ARG	THR	HIS	LEU	HIS	HIS	ALA	GLU	SER	A121	T122	R126	G127	V128	F129	T139	L141	Y142	Y143	P144	M145	E146	L147	G148	R149	R156	I157	V158	L161	L167	K168	R169	A170	V171	W175	P176	N177	H178	E179	I180	I181	L185	L186	V187	P188	Q195	R199	M200	R206	S207	L208	D209	W210	S211	F212	C213	W214	E220	E224	R228	K236	P237	K239	Y242	E243	E244	A245	ARG	THR	HIS	LEU	HIS	HIS	ALA	GLU	SER	A121	T122	R126	G127	V128	F129	T139	L141	Y142	Y143	P144	M145	E146	L147	G148	R149	R156	I157	V158	L161	L167	K168	R169	A170	V171	W175	P176	N177	H178	E179	I180	I181	L185	L186	V187	P188	Q195	R199	M200	R206	S207	L208	D209	W210	S211	F212	C213	W214	E220	E224	R228	K236	P237	K239	Y242	E243	E244	A245	ARG	THR	HIS	LEU	HIS	HIS	ALA	GLU	SER	A121	T122	R126	G127	V128	F129	T139	L141	Y142	Y143	P144	M145	E146	L147	G148	R149	R156	I157	V158	L161	L167	K168	R169	A170	V171	W175	P176	N177	H178
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- Chain J: 69% 22% 5%

[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	76.20Å 103.35Å 104.63Å 105.79° 105.19° 92.68°	Depositor
Resolution (Å)	19.99 – 2.40 49.48 – 2.39	Depositor EDS
% Data completeness (in resolution range)	86.8 (19.99-2.40) 80.1 (49.48-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.153 , 0.229 0.160 , 0.158	Depositor DCC
R_{free} test set	5067 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 100947 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19878	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	1.16	1/1984 (0.1%)	1.08	7/2696 (0.3%)
1	B	1.17	3/1995 (0.2%)	1.13	12/2711 (0.4%)
1	C	1.16	5/1990 (0.3%)	1.12	10/2704 (0.4%)
1	D	1.12	3/1984 (0.2%)	1.08	6/2696 (0.2%)
1	E	1.22	7/1984 (0.4%)	1.13	12/2696 (0.4%)
1	F	1.26	15/1984 (0.8%)	1.13	15/2696 (0.6%)
1	G	1.15	5/1984 (0.3%)	1.05	5/2696 (0.2%)
1	H	1.19	8/1984 (0.4%)	1.08	7/2696 (0.3%)
1	I	1.11	3/1984 (0.2%)	1.08	9/2696 (0.3%)
1	J	1.12	2/1984 (0.1%)	1.03	6/2696 (0.2%)
All	All	1.17	52/19857 (0.3%)	1.09	89/26983 (0.3%)

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	183	GLU	CD-OE2	10.14	1.36	1.25
1	H	225	GLU	CG-CD	8.59	1.64	1.51
1	F	62	GLU	CG-CD	8.18	1.64	1.51
1	F	225	GLU	CG-CD	7.85	1.63	1.51
1	E	225	GLU	CG-CD	7.60	1.63	1.51

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	206	ARG	NE-CZ-NH1	11.66	126.13	120.30
1	C	206	ARG	NE-CZ-NH1	10.83	125.72	120.30
1	C	126	ARG	NE-CZ-NH1	10.80	125.70	120.30
1	E	228	ARG	NE-CZ-NH1	10.50	125.55	120.30
1	B	149	ARG	NE-CZ-NH2	-9.89	115.36	120.30

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	1932	0	1924	58	0
1	B	1942	0	1931	69	0
1	C	1938	0	1929	63	0
1	D	1932	0	1924	48	0
1	E	1932	0	1924	63	0
1	F	1932	0	1924	55	1
1	G	1932	0	1924	64	0
1	H	1932	0	1924	60	1
1	I	1932	0	1924	54	0
1	J	1932	0	1924	44	0
2	A	57	0	0	0	0
2	B	60	0	0	2	0
2	C	39	0	0	4	0
2	D	57	0	0	4	0
2	E	65	0	0	9	0
2	F	59	0	0	6	0
2	G	61	0	0	5	0
2	H	65	0	0	6	0
2	I	30	0	0	2	0
2	J	49	0	0	1	0
All	All	19878	0	19252	524	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 14.

The worst 5 of 524 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:F:206:ARG:HG3	1:F:206:ARG:HH11	1.10	1.15
1:A:123:HIS:HA	1:A:145:MET:HE1	1.33	1.10
1:I:129:PHE:CE2	1:I:140:MET:HE3	1.88	1.08
1:A:206:ARG:HG3	1:A:206:ARG:HH11	1.18	1.07
1:E:220:ARG:HH11	1:E:220:ARG:HG2	0.96	1.06

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:228:ARG:NH1	1:H:228:ARG:CB[1_544]	2.19	0.01

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	234/250 (94%)	224 (96%)	7 (3%)	3 (1%)	15	21
1	B	235/250 (94%)	228 (97%)	6 (3%)	1 (0%)	39	56
1	C	235/250 (94%)	219 (93%)	15 (6%)	1 (0%)	39	56
1	D	234/250 (94%)	219 (94%)	13 (6%)	2 (1%)	21	30
1	E	234/250 (94%)	223 (95%)	11 (5%)	0	100	100
1	F	234/250 (94%)	224 (96%)	8 (3%)	2 (1%)	21	30
1	G	234/250 (94%)	217 (93%)	15 (6%)	2 (1%)	21	30
1	H	234/250 (94%)	221 (94%)	10 (4%)	3 (1%)	15	21
1	I	234/250 (94%)	221 (94%)	10 (4%)	3 (1%)	15	21
1	J	234/250 (94%)	211 (90%)	21 (9%)	2 (1%)	21	30
All	All	2342/2500 (94%)	2207 (94%)	116 (5%)	19 (1%)	24	35

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	THR
1	C	121	ALA
1	F	32	SER
1	F	122	THR
1	I	122	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	206/216 (95%)	189 (92%)	17 (8%)	14	21
1	B	207/216 (96%)	182 (88%)	25 (12%)	6	8
1	C	207/216 (96%)	191 (92%)	16 (8%)	16	24
1	D	206/216 (95%)	188 (91%)	18 (9%)	13	19
1	E	206/216 (95%)	185 (90%)	21 (10%)	9	13
1	F	206/216 (95%)	188 (91%)	18 (9%)	13	19
1	G	206/216 (95%)	191 (93%)	15 (7%)	17	27
1	H	206/216 (95%)	185 (90%)	21 (10%)	9	13
1	I	206/216 (95%)	188 (91%)	18 (9%)	13	19
1	J	206/216 (95%)	190 (92%)	16 (8%)	16	24
All	All	2062/2160 (96%)	1877 (91%)	185 (9%)	12	17

5 of 185 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	145	MET
1	F	145	MET
1	J	41	SER
1	E	161	LEU
1	E	208	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	106	GLN
1	F	106	GLN
1	I	92	HIS
1	E	21	HIS
1	G	106	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	238/250 (95%)	-0.71	2 (0%) 87 87	12, 22, 45, 72	0
1	B	239/250 (95%)	-0.59	0 100 100	14, 24, 44, 62	0
1	C	239/250 (95%)	-0.55	0 100 100	15, 25, 44, 71	0
1	D	238/250 (95%)	-0.62	1 (0%) 93 93	13, 25, 46, 76	0
1	E	238/250 (95%)	-0.55	3 (1%) 79 79	13, 25, 44, 65	0
1	F	238/250 (95%)	-0.66	0 100 100	11, 22, 41, 65	0
1	G	238/250 (95%)	-0.58	0 100 100	14, 24, 44, 59	0
1	H	238/250 (95%)	-0.64	0 100 100	13, 24, 45, 63	0
1	I	238/250 (95%)	-0.53	2 (0%) 87 87	18, 30, 49, 68	0
1	J	238/250 (95%)	-0.65	1 (0%) 93 93	15, 27, 48, 63	0
All	All	2382/2500 (95%)	-0.61	9 (0%) 93 93	11, 25, 46, 76	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	238	ALA	4.7
1	A	245	ALA	3.0
1	A	244	GLU	2.9
1	E	244	GLU	2.5
1	E	242	TYR	2.5

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 [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.