



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:43 AM GMT

PDB ID : 2NVL
Title : Crystal structure of archaeal peroxiredoxin, thioredoxin peroxidase from *Aeropyrum pernix* K1 (sulfonic acid form)
Authors : Nakamura, T.; Yamamoto, T.; Abe, M.; Matsumura, H.; Hagihara, Y.; Goto, T.; Yamaguchi, T.; Inoue, T.
Deposited on : 2006-11-13
Resolution : 2.36 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

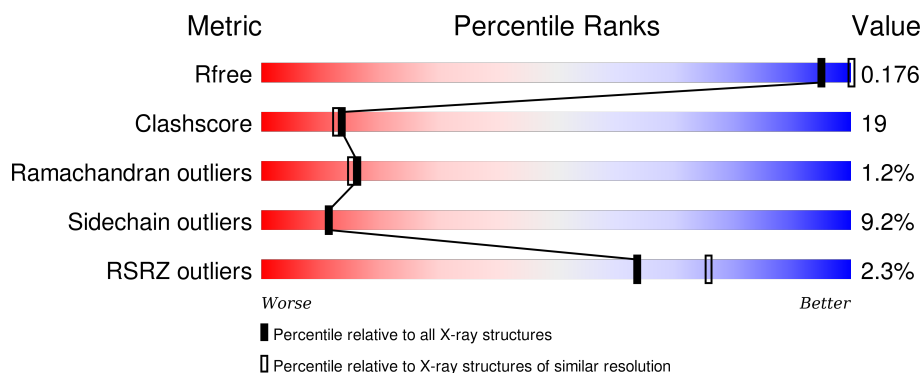
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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>3%</div> <div> <div></div> <div>63%</div> <div>25%</div> <div>8%</div> <div>• •</div> </div> </div>
1	B	250	<div> <div>%</div> <div> <div></div> <div>68%</div> <div>22%</div> <div>5%</div> <div>• •</div> </div> </div>
1	C	250	<div> <div>2%</div> <div> <div></div> <div>63%</div> <div>26%</div> <div>7%</div> <div>•</div> </div> </div>
1	D	250	<div> <div>2%</div> <div> <div></div> <div>62%</div> <div>28%</div> <div>6%</div> <div>• •</div> </div> </div>
1	E	250	<div> <div>2%</div> <div> <div></div> <div>62%</div> <div>29%</div> <div>5%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain	
1	F	250	<div> <div></div> <div>3%</div> <div>62%</div> <div>29%</div> <div>• • •</div> </div>	
1	G	250	<div> <div></div> <div>%</div> <div>62%</div> <div>30%</div> <div>• • •</div> </div>	
1	H	250	<div> <div></div> <div>2%</div> <div>70%</div> <div>20%</div> <div>6%</div> <div>• •</div> </div>	
1	I	250	<div> <div></div> <div>4%</div> <div>62%</div> <div>28%</div> <div>6%</div> <div>• •</div> </div>	
1	J	250	<div> <div></div> <div>2%</div> <div>69%</div> <div>20%</div> <div>6%</div> <div>• •</div> </div>	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20328 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	242	Total	C	N	O	S	0	0	0
			1965	1261	345	353	6			
1	B	240	Total	C	N	O	S	0	0	0
			1953	1254	343	350	6			
1	C	240	Total	C	N	O	S	0	0	0
			1950	1252	341	351	6			
1	D	242	Total	C	N	O	S	0	0	0
			1965	1261	345	353	6			
1	E	242	Total	C	N	O	S	0	0	0
			1965	1261	345	353	6			
1	F	242	Total	C	N	O	S	0	0	0
			1965	1261	345	353	6			
1	G	242	Total	C	N	O	S	0	0	0
			1965	1261	345	353	6			
1	H	242	Total	C	N	O	S	0	0	0
			1965	1261	345	353	6			
1	I	242	Total	C	N	O	S	0	0	0
			1965	1261	345	353	6			
1	J	242	Total	C	N	O	S	0	0	0
			1965	1261	345	353	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

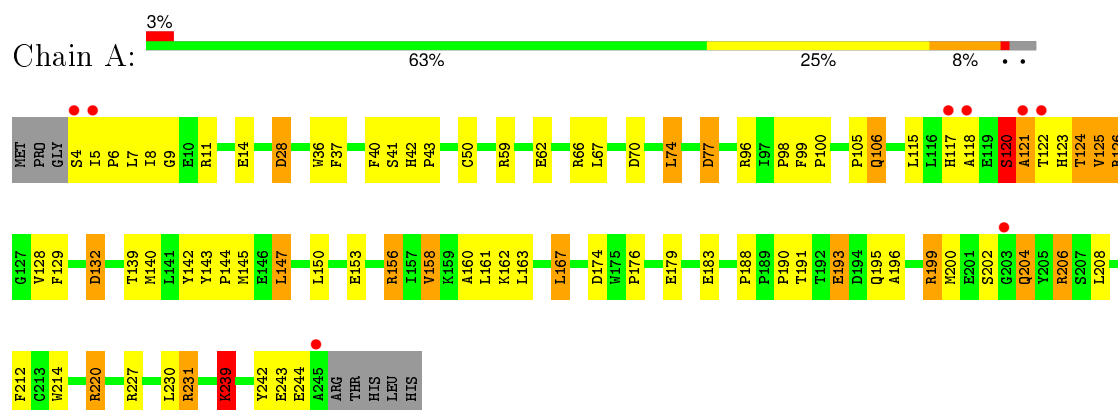
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	83	Total O 83 83	0	0
2	B	64	Total O 64 64	0	0
2	C	58	Total O 58 58	0	0
2	D	44	Total O 44 44	0	0
2	E	66	Total O 66 66	0	0
2	F	75	Total O 75 75	0	0
2	G	82	Total O 82 82	0	0
2	H	82	Total O 82 82	0	0
2	I	75	Total O 75 75	0	0
2	J	76	Total O 76 76	0	0

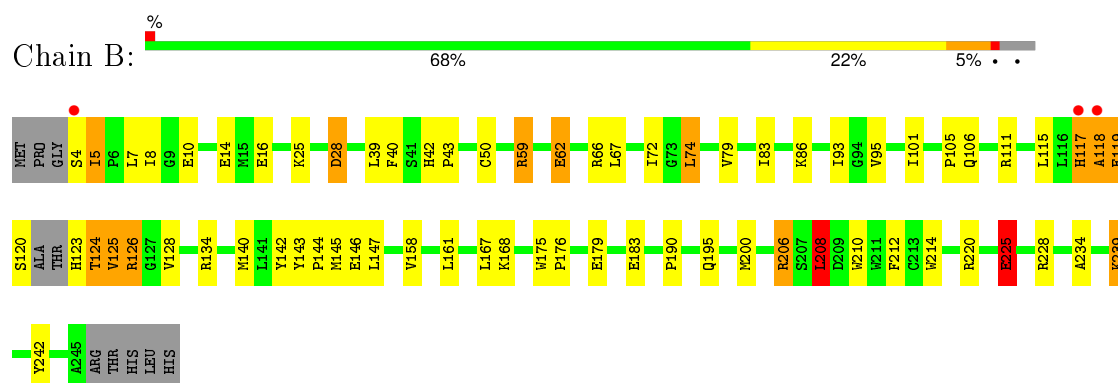
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($\text{RSRZ} > 2$). 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.

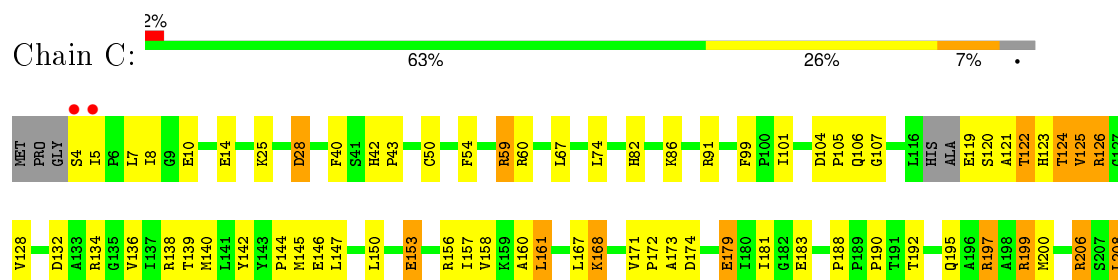
• Molecule 1: Probable peroxiredoxin

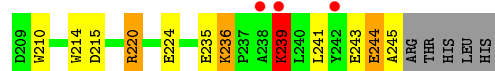


• Molecule 1: Probable peroxiredoxin

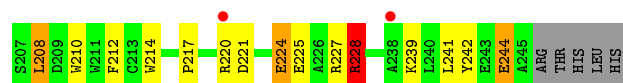
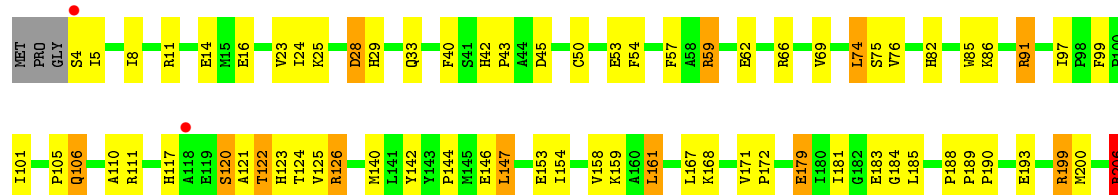


• Molecule 1: Probable peroxiredoxin

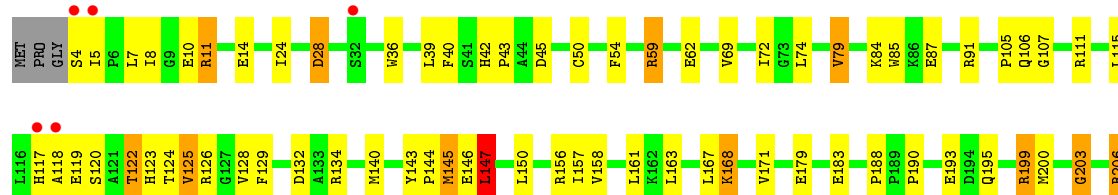




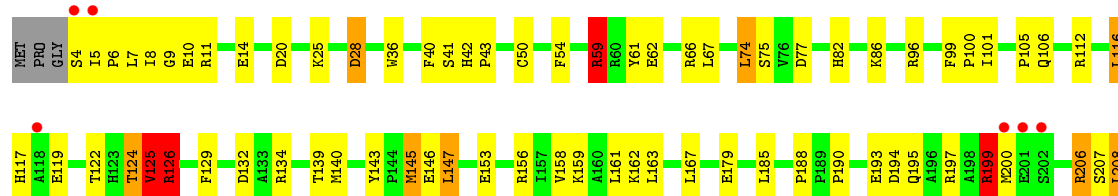
- Molecule 1: Probable peroxiredoxin



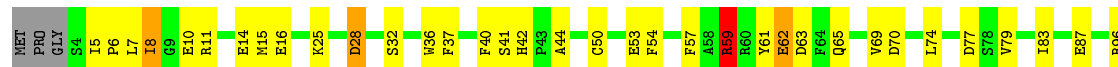
- Molecule 1: Probable peroxiredoxin

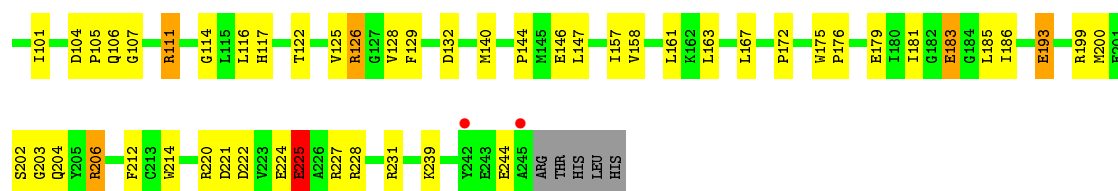


- Molecule 1: Probable peroxiredoxin

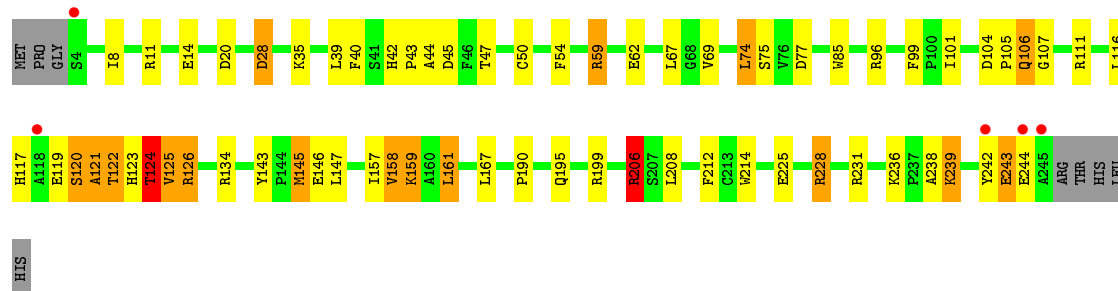


- Molecule 1: Probable peroxiredoxin

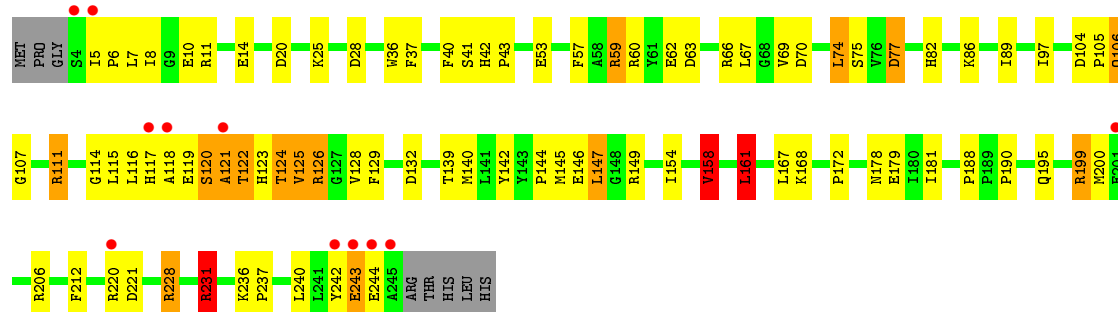




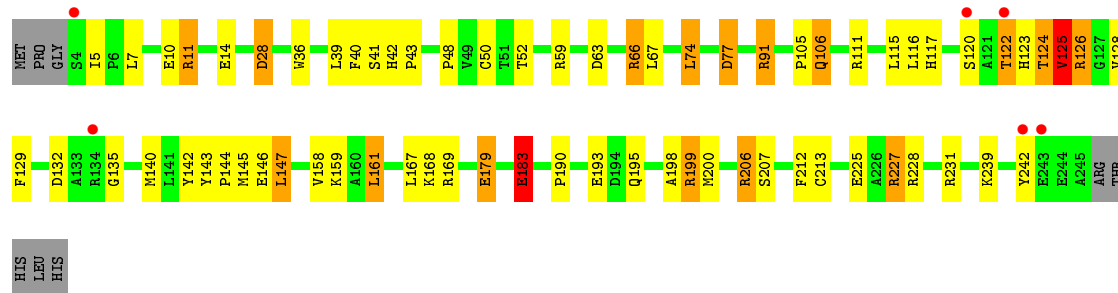
• Molecule 1: Probable peroxiredoxin



• Molecule 1: Probable peroxiredoxin



• Molecule 1: Probable peroxiredoxin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	76.32Å 102.96Å 104.30Å 105.65° 105.26° 92.69°	Depositor
Resolution (Å)	50.00 – 2.36 50.13 – 2.36	Depositor EDS
% Data completeness (in resolution range)	96.5 (50.00-2.36) 84.9 (50.13-2.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.166 , 0.219 0.167 , 0.176	Depositor DCC
R_{free} test set	11666 reflections (11.70%)	DCC
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 116808 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20328	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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

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

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	1.19	3/2009 (0.1%)	1.04	8/2730 (0.3%)
1	B	1.20	6/1996 (0.3%)	1.02	5/2710 (0.2%)
1	C	1.17	4/1992 (0.2%)	1.00	7/2705 (0.3%)
1	D	1.13	5/2009 (0.2%)	1.02	8/2730 (0.3%)
1	E	1.18	5/2009 (0.2%)	1.02	7/2730 (0.3%)
1	F	1.22	3/2009 (0.1%)	1.11	17/2730 (0.6%)
1	G	1.28	10/2009 (0.5%)	1.09	11/2730 (0.4%)
1	H	1.17	3/2009 (0.1%)	1.06	7/2730 (0.3%)
1	I	1.16	5/2009 (0.2%)	1.04	12/2730 (0.4%)
1	J	1.17	5/2009 (0.2%)	1.02	6/2730 (0.2%)
All	All	1.19	49/20060 (0.2%)	1.04	88/27255 (0.3%)

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	1

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	179	GLU	CD-OE1	9.85	1.36	1.25
1	E	183	GLU	CD-OE2	9.63	1.36	1.25
1	G	225	GLU	CG-CD	7.96	1.63	1.51
1	B	225	GLU	CG-CD	7.62	1.63	1.51
1	G	62	GLU	CG-CD	7.53	1.63	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	59	ARG	NE-CZ-NH1	11.61	126.10	120.30
1	J	231	ARG	NE-CZ-NH2	-10.91	114.84	120.30
1	G	126	ARG	NE-CZ-NH2	-10.85	114.87	120.30
1	G	231	ARG	NE-CZ-NH2	-9.71	115.45	120.30
1	F	227	ARG	NE-CZ-NH1	-9.39	115.60	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	SER	Peptide

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	1965	0	1948	93	0
1	B	1953	0	1935	73	0
1	C	1950	0	1935	74	0
1	D	1965	0	1948	99	0
1	E	1965	0	1948	97	0
1	F	1965	0	1948	94	0
1	G	1965	0	1948	70	0
1	H	1965	0	1948	60	0
1	I	1965	0	1948	87	0
1	J	1965	0	1947	84	0
2	A	83	0	0	5	0
2	B	64	0	0	6	0
2	C	58	0	0	6	0
2	D	44	0	0	3	0
2	E	66	0	0	5	0
2	F	75	0	0	5	0
2	G	82	0	0	4	0
2	H	82	0	0	6	0
2	I	75	0	0	3	0
2	J	76	0	0	3	0
All	All	20328	0	19453	727	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 19.

The worst 5 of 727 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:66:ARG:HH11	1:J:66:ARG:HG3	1.05	1.16
1:D:105:PRO:O	1:D:106:GLN:HB3	1.43	1.15
1:G:105:PRO:O	1:G:106:GLN:HB2	1.48	1.13
1:G:14:GLU:HG3	1:G:25:LYS:HZ1	1.00	1.10
1:B:126:ARG:HH11	1:B:145:MET:HA	1.11	1.08

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	239/250 (96%)	221 (92%)	16 (7%)	2 (1%)	24	26
1	B	235/250 (94%)	223 (95%)	9 (4%)	3 (1%)	15	13
1	C	235/250 (94%)	224 (95%)	8 (3%)	3 (1%)	15	13
1	D	239/250 (96%)	226 (95%)	10 (4%)	3 (1%)	15	13
1	E	239/250 (96%)	220 (92%)	15 (6%)	4 (2%)	11	9
1	F	239/250 (96%)	228 (95%)	10 (4%)	1 (0%)	39	46
1	G	239/250 (96%)	227 (95%)	10 (4%)	2 (1%)	24	26
1	H	239/250 (96%)	226 (95%)	8 (3%)	5 (2%)	9	6
1	I	239/250 (96%)	226 (95%)	10 (4%)	3 (1%)	15	13
1	J	239/250 (96%)	223 (93%)	14 (6%)	2 (1%)	24	26
All	All	2382/2500 (95%)	2244 (94%)	110 (5%)	28 (1%)	16	15

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	ALA
1	B	118	ALA
1	C	121	ALA
1	E	239	LYS
1	G	239	LYS

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	208/215 (97%)	188 (90%)	20 (10%)	10	10
1	B	207/215 (96%)	189 (91%)	18 (9%)	13	13
1	C	207/215 (96%)	186 (90%)	21 (10%)	9	9
1	D	208/215 (97%)	188 (90%)	20 (10%)	10	10
1	E	208/215 (97%)	192 (92%)	16 (8%)	16	17
1	F	208/215 (97%)	190 (91%)	18 (9%)	13	13
1	G	208/215 (97%)	192 (92%)	16 (8%)	16	17
1	H	208/215 (97%)	187 (90%)	21 (10%)	9	9
1	I	208/215 (97%)	187 (90%)	21 (10%)	9	9
1	J	208/215 (97%)	188 (90%)	20 (10%)	10	10
All	All	2078/2150 (97%)	1887 (91%)	191 (9%)	11	11

5 of 191 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	145	MET
1	F	193	GLU
1	J	77	ASP
1	E	167	LEU
1	F	59	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	117	HIS
1	G	123	HIS
1	I	117	HIS
1	F	195	GLN
1	G	92	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	OCS	A	50	1	7,8,9	2.92	3 (42%)	7,11,13	1.55	1 (14%)
1	OCS	B	50	1	7,8,9	2.27	3 (42%)	7,11,13	3.80	3 (42%)
1	OCS	C	50	1	7,8,9	2.50	2 (28%)	7,11,13	3.83	4 (57%)
1	OCS	D	50	1	7,8,9	2.91	3 (42%)	7,11,13	2.30	2 (28%)
1	OCS	E	50	1	7,8,9	2.82	2 (28%)	7,11,13	2.60	4 (57%)
1	OCS	F	50	1	7,8,9	2.34	3 (42%)	7,11,13	1.46	1 (14%)
1	OCS	G	50	1	7,8,9	2.46	2 (28%)	7,11,13	1.97	2 (28%)
1	OCS	H	50	1	7,8,9	2.65	2 (28%)	7,11,13	2.48	3 (42%)
1	OCS	I	50	1	7,8,9	3.14	2 (28%)	7,11,13	2.09	4 (57%)
1	OCS	J	50	1	7,8,9	2.77	2 (28%)	7,11,13	2.62	3 (42%)

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
1	OCS	A	50	1	-	0/4/7/9	0/0/0/0
1	OCS	B	50	1	-	0/4/7/9	0/0/0/0
1	OCS	C	50	1	-	0/4/7/9	0/0/0/0
1	OCS	D	50	1	-	0/4/7/9	0/0/0/0
1	OCS	E	50	1	-	0/4/7/9	0/0/0/0
1	OCS	F	50	1	-	0/4/7/9	0/0/0/0
1	OCS	G	50	1	-	0/4/7/9	0/0/0/0
1	OCS	H	50	1	-	0/4/7/9	0/0/0/0
1	OCS	I	50	1	-	0/4/7/9	0/0/0/0
1	OCS	J	50	1	-	0/4/7/9	0/0/0/0

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	50	OCS	CB-SG	-6.86	1.67	1.77
1	H	50	OCS	CB-SG	-6.15	1.68	1.77
1	A	50	OCS	CB-SG	-5.98	1.69	1.77
1	D	50	OCS	CB-SG	-5.94	1.69	1.77
1	E	50	OCS	CB-SG	-5.82	1.69	1.77

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	50	OCS	O-C-CA	-4.82	112.94	125.49
1	J	50	OCS	OD1-SG-CB	-4.81	102.89	106.94
1	B	50	OCS	O-C-CA	-4.48	113.83	125.49
1	E	50	OCS	O-C-CA	-4.31	114.25	125.49
1	C	50	OCS	O-C-CA	-4.31	114.28	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	50	OCS	1	0
1	B	50	OCS	2	0
1	C	50	OCS	2	0
1	D	50	OCS	1	0
1	E	50	OCS	2	0
1	F	50	OCS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	50	OCS	1	0
1	H	50	OCS	1	0
1	J	50	OCS	1	0

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	241/250 (96%)	-0.25	8 (3%)	50	63	19, 30, 60, 79	0
1	B	239/250 (95%)	-0.29	3 (1%)	79	87	21, 31, 59, 79	0
1	C	239/250 (95%)	-0.33	5 (2%)	67	79	22, 33, 61, 74	0
1	D	241/250 (96%)	-0.18	4 (1%)	73	83	25, 38, 63, 79	0
1	E	241/250 (96%)	-0.13	5 (2%)	67	79	19, 33, 62, 78	0
1	F	241/250 (96%)	-0.25	7 (2%)	55	67	20, 29, 57, 72	0
1	G	241/250 (96%)	-0.31	2 (0%)	87	93	18, 28, 54, 73	0
1	H	241/250 (96%)	-0.27	5 (2%)	67	79	19, 28, 59, 78	0
1	I	241/250 (96%)	-0.20	11 (4%)	36	51	20, 31, 63, 83	0
1	J	241/250 (96%)	-0.16	6 (2%)	61	73	22, 32, 59, 76	0
All	All	2406/2500 (96%)	-0.24	56 (2%)	64	76	18, 32, 61, 83	0

The worst 5 of 56 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	118	ALA	7.0
1	I	118	ALA	5.4
1	E	4	SER	5.2
1	H	245	ALA	4.2
1	I	4	SER	4.1

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
1	OCS	J	50	9/10	0.98	0.12	-	27,29,35,35	0
1	OCS	I	50	9/10	0.98	0.10	-	25,26,33,34	0
1	OCS	F	50	9/10	0.97	0.13	-	25,27,33,34	0
1	OCS	E	50	9/10	0.98	0.11	-	27,28,38,38	0
1	OCS	H	50	9/10	0.98	0.10	-	20,21,31,31	0
1	OCS	G	50	9/10	0.98	0.10	-	23,25,29,31	0
1	OCS	B	50	9/10	0.98	0.10	-	23,24,33,33	0
1	OCS	A	50	9/10	0.98	0.10	-	26,28,35,35	0
1	OCS	D	50	9/10	0.98	0.08	-	28,30,36,41	0
1	OCS	C	50	9/10	0.98	0.09	-	26,27,33,33	0

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.