



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:05 am BST

PDB ID : 5ZTE
Title : Crystal structure of PrxA C119S mutant from Arabidopsis thaliana
Authors : Yang, Y.; Cai, W.; Wang, J.; Pan, W.; Liu, L.; Wang, M.; Zhang, M.
Deposited on : 2018-05-03
Resolution : 2.60 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
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

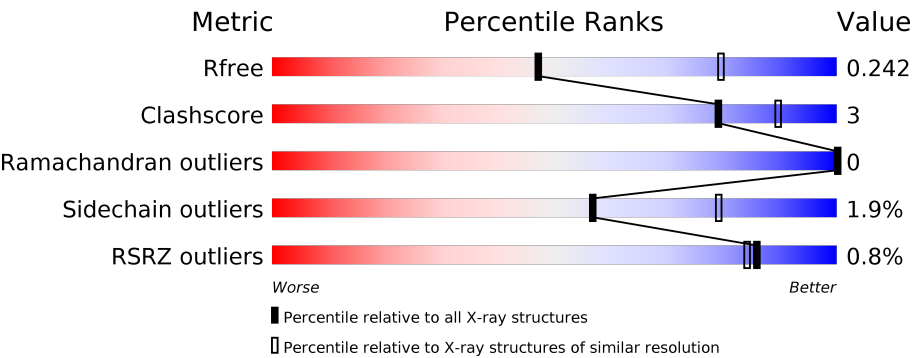
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	203	<div><div></div><div>89%7%.</div></div>
1	B	203	<div><div></div><div>87%11%.</div></div>
1	C	203	<div><div></div><div>85%10%5%</div></div>
1	D	203	<div><div>%</div><div>91%5%.</div></div>
1	E	203	<div><div>%</div><div>84%10%. .</div></div>
1	F	203	<div><div></div><div>94%. .</div></div>

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Mol	Chain	Length	Quality of chain
1	G	203	<div><div><div>%</div><div><div></div><div>86%</div><div>6%</div><div>8%</div></div></div></div>
1	H	203	<div><div><div></div><div>86%</div><div>9%</div><div>5%</div></div></div>
1	I	203	<div><div><div>2%</div><div><div></div><div>88%</div><div>7%</div><div>•</div></div></div></div>
1	J	203	<div><div><div>%</div><div><div></div><div>82%</div><div>13%</div><div>•</div></div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15830 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 2-Cys peroxiredoxin BAS1, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	0	0	0
			1540	995	248	294	3			
1	B	198	Total	C	N	O	S	0	0	0
			1575	1013	261	298	3			
1	C	193	Total	C	N	O	S	0	0	0
			1524	983	246	292	3			
1	D	195	Total	C	N	O	S	0	0	0
			1540	995	248	294	3			
1	E	194	Total	C	N	O	S	0	0	0
			1532	989	247	293	3			
1	F	196	Total	C	N	O	S	0	0	0
			1549	1000	249	297	3			
1	G	187	Total	C	N	O	S	0	0	0
			1472	948	239	282	3			
1	H	193	Total	C	N	O	S	0	0	0
			1524	983	246	292	3			
1	I	194	Total	C	N	O	S	0	0	0
			1532	989	247	293	3			
1	J	194	Total	C	N	O	S	0	0	0
			1532	989	247	293	3			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	MET	-	expression tag	UNP Q96291
A	119	SER	CYS	engineered mutation	UNP Q96291
A	267	LEU	-	expression tag	UNP Q96291
A	268	GLU	-	expression tag	UNP Q96291
A	269	HIS	-	expression tag	UNP Q96291
A	270	HIS	-	expression tag	UNP Q96291
A	271	HIS	-	expression tag	UNP Q96291
A	272	HIS	-	expression tag	UNP Q96291
A	273	HIS	-	expression tag	UNP Q96291

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Chain	Residue	Modelled	Actual	Comment	Reference
A	274	HIS	-	expression tag	UNP Q96291
B	72	MET	-	expression tag	UNP Q96291
B	119	SER	CYS	engineered mutation	UNP Q96291
B	267	LEU	-	expression tag	UNP Q96291
B	268	GLU	-	expression tag	UNP Q96291
B	269	HIS	-	expression tag	UNP Q96291
B	270	HIS	-	expression tag	UNP Q96291
B	271	HIS	-	expression tag	UNP Q96291
B	272	HIS	-	expression tag	UNP Q96291
B	273	HIS	-	expression tag	UNP Q96291
B	274	HIS	-	expression tag	UNP Q96291
C	72	MET	-	expression tag	UNP Q96291
C	119	SER	CYS	engineered mutation	UNP Q96291
C	267	LEU	-	expression tag	UNP Q96291
C	268	GLU	-	expression tag	UNP Q96291
C	269	HIS	-	expression tag	UNP Q96291
C	270	HIS	-	expression tag	UNP Q96291
C	271	HIS	-	expression tag	UNP Q96291
C	272	HIS	-	expression tag	UNP Q96291
C	273	HIS	-	expression tag	UNP Q96291
C	274	HIS	-	expression tag	UNP Q96291
D	72	MET	-	expression tag	UNP Q96291
D	119	SER	CYS	engineered mutation	UNP Q96291
D	267	LEU	-	expression tag	UNP Q96291
D	268	GLU	-	expression tag	UNP Q96291
D	269	HIS	-	expression tag	UNP Q96291
D	270	HIS	-	expression tag	UNP Q96291
D	271	HIS	-	expression tag	UNP Q96291
D	272	HIS	-	expression tag	UNP Q96291
D	273	HIS	-	expression tag	UNP Q96291
D	274	HIS	-	expression tag	UNP Q96291
E	72	MET	-	expression tag	UNP Q96291
E	119	SER	CYS	engineered mutation	UNP Q96291
E	267	LEU	-	expression tag	UNP Q96291
E	268	GLU	-	expression tag	UNP Q96291
E	269	HIS	-	expression tag	UNP Q96291
E	270	HIS	-	expression tag	UNP Q96291
E	271	HIS	-	expression tag	UNP Q96291
E	272	HIS	-	expression tag	UNP Q96291
E	273	HIS	-	expression tag	UNP Q96291
E	274	HIS	-	expression tag	UNP Q96291
F	72	MET	-	expression tag	UNP Q96291

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Chain	Residue	Modelled	Actual	Comment	Reference
F	119	SER	CYS	engineered mutation	UNP Q96291
F	267	LEU	-	expression tag	UNP Q96291
F	268	GLU	-	expression tag	UNP Q96291
F	269	HIS	-	expression tag	UNP Q96291
F	270	HIS	-	expression tag	UNP Q96291
F	271	HIS	-	expression tag	UNP Q96291
F	272	HIS	-	expression tag	UNP Q96291
F	273	HIS	-	expression tag	UNP Q96291
F	274	HIS	-	expression tag	UNP Q96291
G	72	MET	-	expression tag	UNP Q96291
G	119	SER	CYS	engineered mutation	UNP Q96291
G	267	LEU	-	expression tag	UNP Q96291
G	268	GLU	-	expression tag	UNP Q96291
G	269	HIS	-	expression tag	UNP Q96291
G	270	HIS	-	expression tag	UNP Q96291
G	271	HIS	-	expression tag	UNP Q96291
G	272	HIS	-	expression tag	UNP Q96291
G	273	HIS	-	expression tag	UNP Q96291
G	274	HIS	-	expression tag	UNP Q96291
H	72	MET	-	expression tag	UNP Q96291
H	119	SER	CYS	engineered mutation	UNP Q96291
H	267	LEU	-	expression tag	UNP Q96291
H	268	GLU	-	expression tag	UNP Q96291
H	269	HIS	-	expression tag	UNP Q96291
H	270	HIS	-	expression tag	UNP Q96291
H	271	HIS	-	expression tag	UNP Q96291
H	272	HIS	-	expression tag	UNP Q96291
H	273	HIS	-	expression tag	UNP Q96291
H	274	HIS	-	expression tag	UNP Q96291
I	72	MET	-	expression tag	UNP Q96291
I	119	SER	CYS	engineered mutation	UNP Q96291
I	267	LEU	-	expression tag	UNP Q96291
I	268	GLU	-	expression tag	UNP Q96291
I	269	HIS	-	expression tag	UNP Q96291
I	270	HIS	-	expression tag	UNP Q96291
I	271	HIS	-	expression tag	UNP Q96291
I	272	HIS	-	expression tag	UNP Q96291
I	273	HIS	-	expression tag	UNP Q96291
I	274	HIS	-	expression tag	UNP Q96291
J	72	MET	-	expression tag	UNP Q96291
J	119	SER	CYS	engineered mutation	UNP Q96291
J	267	LEU	-	expression tag	UNP Q96291

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Chain	Residue	Modelled	Actual	Comment	Reference
J	268	GLU	-	expression tag	UNP Q96291
J	269	HIS	-	expression tag	UNP Q96291
J	270	HIS	-	expression tag	UNP Q96291
J	271	HIS	-	expression tag	UNP Q96291
J	272	HIS	-	expression tag	UNP Q96291
J	273	HIS	-	expression tag	UNP Q96291
J	274	HIS	-	expression tag	UNP Q96291

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	62	Total 62	O 62	0	0
2	B	58	Total 58	O 58	0	0
2	C	44	Total 44	O 44	0	0
2	D	32	Total 32	O 32	0	0
2	E	33	Total 33	O 33	0	0
2	F	83	Total 83	O 83	0	0
2	G	71	Total 71	O 71	0	0
2	H	36	Total 36	O 36	0	0
2	I	50	Total 50	O 50	0	0
2	J	41	Total 41	O 41	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 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: 2-Cys peroxiredoxin BAS1, chloroplastic

Chain A: 




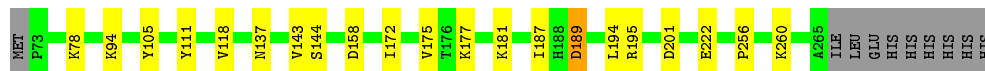
- Molecule 1: 2-Cys peroxiredoxin BAS1, chloroplastic

Chain B: 

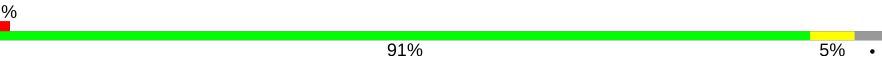


- Molecule 1: 2-Cys peroxiredoxin BAS1, chloroplastic

Chain C: 




- Molecule 1: 2-Cys peroxiredoxin BAS1, chloroplastic

Chain D: 



- Molecule 1: 2-Cys peroxiredoxin BAS1, chloroplastic

Chain E: 



- Molecule 1: 2-Cys peroxiredoxin BAS1, chloroplastic

Diagram illustrating the protein structure of the C-terminal domain of the human protein, showing conserved residues (green) and non-conserved residues (yellow).

Conserved residues (green): P73, Y105, V118, V175, T176, K177, R195, D201, E268.

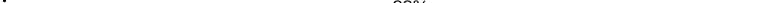
Non-conserved residues (yellow): MET, P73, Y105, V118, V175, T176, K177, R195, D201, E268, HIS.

- Chain G: 86% 6% 8%

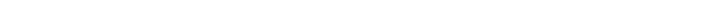


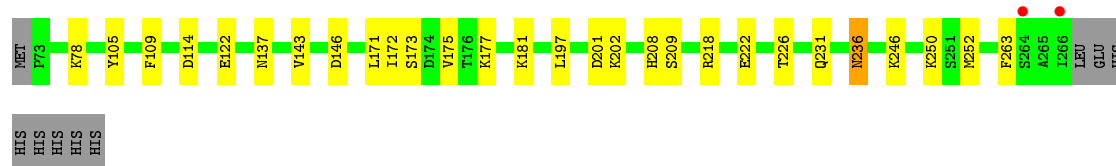
- Chain H: 86% 9% 5%



- Chain I:  2% 88% 7%



- Chain J:  82% 13% .



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	124.21Å 216.19Å 98.45Å 90.00° 101.47° 90.00°	Depositor
Resolution (Å)	40.74 – 2.60 47.10 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.5 (40.74-2.60) 95.7 (47.10-2.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.61Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.196 , 0.244 0.196 , 0.242	Depositor DCC
R_{free} test set	3770 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15830	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.89 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5618e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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](#)

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	0.36	0/1576	0.56	0/2133
1	B	0.34	0/1615	0.55	0/2183
1	C	0.34	0/1560	0.51	0/2111
1	D	0.35	0/1576	0.54	0/2133
1	E	0.34	0/1568	0.52	0/2122
1	F	0.36	0/1585	0.55	0/2145
1	G	0.37	0/1506	0.56	0/2039
1	H	0.36	0/1560	0.53	0/2111
1	I	0.33	0/1568	0.53	0/2122
1	J	0.34	0/1568	0.51	0/2122
All	All	0.35	0/15682	0.54	0/21221

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1540	0	1531	8	0
1	B	1575	0	1540	13	0
1	C	1524	0	1509	11	0
1	D	1540	0	1531	8	0
1	E	1532	0	1520	12	1
1	F	1549	0	1537	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1472	0	1462	8	0
1	H	1524	0	1509	12	0
1	I	1532	0	1520	11	0
1	J	1532	0	1520	16	1
2	A	62	0	0	0	1
2	B	58	0	0	1	0
2	C	44	0	0	1	0
2	D	32	0	0	0	0
2	E	33	0	0	0	0
2	F	83	0	0	0	1
2	G	71	0	0	0	0
2	H	36	0	0	1	0
2	I	50	0	0	1	0
2	J	41	0	0	1	0
All	All	15830	0	15179	86	3

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 3.

All (86) 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:C:177:LYS:NZ	1:D:175:VAL:O	2.07	0.87
1:H:177:LYS:NZ	1:I:175:VAL:O	2.08	0.87
1:C:175:VAL:O	1:D:177:LYS:NZ	2.15	0.79
1:A:175:VAL:O	1:B:177:LYS:NZ	2.16	0.78
1:F:175:VAL:O	1:G:177:LYS:NZ	2.18	0.76
1:H:175:VAL:O	1:I:177:LYS:NZ	2.19	0.73
1:I:222:GLU:HG2	1:J:222:GLU:HG2	1.74	0.67
1:J:137:ASN:HD22	1:J:202:LYS:HE2	1.58	0.67
1:C:143:VAL:HG22	1:C:172:ILE:HB	1.77	0.66
1:B:222:GLU:HG2	1:C:222:GLU:HG2	1.77	0.66
1:J:246:LYS:NZ	2:J:301:HOH:O	2.29	0.65
1:I:104:LYS:NZ	2:I:302:HOH:O	2.29	0.65
1:D:222:GLU:HG2	1:E:222:GLU:HG2	1.79	0.65
1:H:222:GLU:OE1	2:H:301:HOH:O	2.15	0.64
1:G:222:GLU:HG2	1:H:222:GLU:HG2	1.79	0.64
1:I:177:LYS:HZ3	1:I:191:GLY:HA3	1.63	0.62
1:J:143:VAL:HG22	1:J:172:ILE:HB	1.81	0.62
1:F:177:LYS:NZ	1:G:175:VAL:O	2.34	0.60
1:A:177:LYS:NZ	1:B:175:VAL:O	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:257:LYS:HG2	1:I:91:GLU:HG2	1.85	0.58
1:J:137:ASN:ND2	1:J:202:LYS:HE2	2.22	0.55
1:E:143:VAL:HG22	1:E:172:ILE:HB	1.88	0.54
1:F:105:TYR:CD2	1:F:201:ASP:HA	2.43	0.54
1:A:118:VAL:HB	1:A:195:ARG:NH2	2.23	0.54
1:I:105:TYR:CD2	1:I:201:ASP:HA	2.43	0.54
1:G:105:TYR:CD2	1:G:201:ASP:HA	2.43	0.53
1:B:257:LYS:HG2	1:D:91:GLU:HG2	1.90	0.53
1:J:252:MET:HE1	1:J:263:PHE:CZ	2.45	0.51
1:D:105:TYR:CD2	1:D:201:ASP:HA	2.46	0.50
1:C:94:LYS:NZ	2:C:303:HOH:O	2.38	0.50
1:J:173:SER:OG	1:J:175:VAL:HG23	2.11	0.50
1:H:118:VAL:HB	1:H:195:ARG:NH2	2.27	0.49
1:H:173:SER:OG	1:H:175:VAL:HG23	2.13	0.49
1:H:137:ASN:HD22	1:H:202:LYS:HE3	1.77	0.49
1:G:254:PRO:HB3	1:H:117:PHE:CD2	2.48	0.49
1:C:105:TYR:CD2	1:C:201:ASP:HA	2.48	0.48
1:A:105:TYR:CD2	1:A:201:ASP:HA	2.48	0.48
1:I:252:MET:HE3	1:I:262:TYR:HB3	1.96	0.48
1:B:201:ASP:HB2	2:B:304:HOH:O	2.14	0.47
1:G:173:SER:OG	1:G:175:VAL:HG23	2.15	0.47
1:J:105:TYR:CD2	1:J:201:ASP:HA	2.49	0.47
1:B:252:MET:O	1:B:254:PRO:HD3	2.14	0.46
1:C:111:TYR:CZ	1:C:144:SER:HB3	2.50	0.46
1:J:122:GLU:CD	1:J:218:ARG:HH21	2.18	0.46
1:F:118:VAL:HB	1:F:195:ARG:NH2	2.30	0.46
1:F:177:LYS:HE3	1:G:177:LYS:HE3	1.98	0.46
1:D:253:LYS:HD2	1:D:258:LEU:HD13	1.99	0.45
1:E:122:GLU:CD	1:E:218:ARG:HH21	2.20	0.45
1:D:230:LEU:O	1:D:234:GLN:HG3	2.17	0.45
1:B:262:TYR:OH	1:D:85:GLU:OE2	2.30	0.45
1:J:105:TYR:CZ	1:J:231:GLN:HG2	2.52	0.45
1:E:250:LYS:CE	1:E:250:LYS:H	2.30	0.45
1:B:103:LYS:HD3	1:H:237:PRO:HG3	1.96	0.45
1:C:118:VAL:HB	1:C:195:ARG:NH2	2.32	0.45
1:E:154:TRP:CE3	1:E:164:LEU:HD11	2.51	0.45
1:E:105:TYR:CD2	1:E:201:ASP:HA	2.51	0.45
1:E:246:LYS:H	1:E:249:GLU:HG3	1.81	0.45
1:B:242:PRO:HG3	1:B:252:MET:HG3	1.98	0.44
1:J:252:MET:HE1	1:J:263:PHE:CE2	2.53	0.44
1:E:250:LYS:H	1:E:250:LYS:CD	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:ASP:OD1	1:C:189:ASP:N	2.45	0.43
1:I:141:LEU:HD22	1:I:172:ILE:HD11	1.99	0.43
1:A:173:SER:OG	1:A:175:VAL:HG23	2.18	0.43
1:B:260:LYS:HA	1:B:263:PHE:HB3	2.01	0.43
1:I:104:LYS:HB3	1:I:104:LYS:HE2	1.84	0.43
1:B:105:TYR:CD2	1:B:201:ASP:HA	2.53	0.43
1:J:109:PHE:HB3	1:J:197:LEU:HD12	2.01	0.43
1:H:105:TYR:CD2	1:H:201:ASP:HA	2.54	0.42
1:A:197:LEU:O	1:A:209:SER:HA	2.20	0.42
1:C:187:ILE:HD11	1:C:194:LEU:CD2	2.49	0.42
1:J:114:ASP:N	1:J:146:ASP:OD2	2.41	0.42
1:A:197:LEU:N	1:A:210:THR:O	2.44	0.42
1:E:114:ASP:N	1:E:146:ASP:OD2	2.48	0.42
1:I:111:TYR:CZ	1:I:144:SER:HB3	2.55	0.42
1:J:171:LEU:HA	1:J:171:LEU:HD23	1.92	0.42
1:E:236:ASN:OD1	1:E:236:ASN:N	2.53	0.41
1:C:256:PRO:O	1:C:260:LYS:HE2	2.20	0.41
1:A:123:ILE:HG22	1:A:167:LEU:HD21	2.03	0.41
1:H:140:VAL:O	1:H:169:TYR:HB2	2.20	0.41
1:H:253:LYS:HD2	1:H:258:LEU:HD13	2.02	0.41
1:E:105:TYR:CZ	1:E:231:GLN:HG2	2.56	0.41
1:E:173:SER:OG	1:E:175:VAL:HG23	2.21	0.41
1:J:208:HIS:CG	1:J:226:THR:HG21	2.56	0.41
1:B:167:LEU:HD12	1:B:171:LEU:HG	2.03	0.40
1:B:118:VAL:HB	1:B:195:ARG:NH2	2.36	0.40
1:J:236:ASN:N	1:J:236:ASN:OD1	2.55	0.40

All (3) 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:J:175:VAL:O	1:J:177:LYS:NZ[2_655]	2.13	0.07
1:E:175:VAL:O	1:E:177:LYS:NZ[2_656]	2.15	0.05
2:A:302:HOH:O	2:F:355:HOH:O[2_656]	2.18	0.02

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	193/203 (95%)	189 (98%)	4 (2%)	0	100	100
1	B	194/203 (96%)	187 (96%)	7 (4%)	0	100	100
1	C	191/203 (94%)	185 (97%)	6 (3%)	0	100	100
1	D	193/203 (95%)	185 (96%)	8 (4%)	0	100	100
1	E	192/203 (95%)	186 (97%)	6 (3%)	0	100	100
1	F	194/203 (96%)	190 (98%)	4 (2%)	0	100	100
1	G	185/203 (91%)	179 (97%)	6 (3%)	0	100	100
1	H	191/203 (94%)	185 (97%)	6 (3%)	0	100	100
1	I	192/203 (95%)	185 (96%)	7 (4%)	0	100	100
1	J	192/203 (95%)	187 (97%)	5 (3%)	0	100	100
All	All	1917/2030 (94%)	1858 (97%)	59 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	172/180 (96%)	170 (99%)	2 (1%)	71	87
1	B	175/180 (97%)	170 (97%)	5 (3%)	42	68
1	C	170/180 (94%)	165 (97%)	5 (3%)	42	68
1	D	172/180 (96%)	172 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	171/180 (95%)	165 (96%)	6 (4%)	36	62
1	F	173/180 (96%)	173 (100%)	0	100	100
1	G	165/180 (92%)	161 (98%)	4 (2%)	49	74
1	H	170/180 (94%)	167 (98%)	3 (2%)	59	80
1	I	171/180 (95%)	168 (98%)	3 (2%)	59	80
1	J	171/180 (95%)	166 (97%)	5 (3%)	42	68
All	All	1710/1800 (95%)	1677 (98%)	33 (2%)	57	79

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	ASP
1	A	236	ASN
1	B	89	ASP
1	B	181	LYS
1	B	189	ASP
1	B	236	ASN
1	B	273	HIS
1	C	78	LYS
1	C	137	ASN
1	C	158	ASP
1	C	181	LYS
1	C	189	ASP
1	E	104	LYS
1	E	181	LYS
1	E	189	ASP
1	E	236	ASN
1	E	250	LYS
1	E	266	ILE
1	G	89	ASP
1	G	137	ASN
1	G	189	ASP
1	G	209	SER
1	H	203	GLU
1	H	238	ASP
1	H	260	LYS
1	I	89	ASP
1	I	104	LYS
1	I	181	LYS
1	J	78	LYS

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Mol	Chain	Res	Type
1	J	181	LYS
1	J	209	SER
1	J	236	ASN
1	J	250	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	273	HIS
1	B	274	HIS
1	H	137	ASN
1	J	137	ASN

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	195/203 (96%)	-0.53	0 100 100	25, 33, 49, 58	0
1	B	198/203 (97%)	-0.37	0 100 100	25, 35, 65, 94	0
1	C	193/203 (95%)	-0.36	0 100 100	25, 37, 57, 71	0
1	D	195/203 (96%)	-0.38	3 (1%) 73 70	27, 37, 61, 73	0
1	E	194/203 (95%)	-0.28	2 (1%) 82 80	30, 41, 63, 72	0
1	F	196/203 (96%)	-0.50	0 100 100	24, 32, 50, 75	0
1	G	187/203 (92%)	-0.43	2 (1%) 80 78	24, 33, 64, 94	0
1	H	193/203 (95%)	-0.22	1 (0%) 91 89	28, 40, 60, 72	0
1	I	194/203 (95%)	-0.29	5 (2%) 56 50	28, 39, 64, 81	0
1	J	194/203 (95%)	-0.34	2 (1%) 82 80	28, 39, 63, 77	0
All	All	1939/2030 (95%)	-0.37	15 (0%) 86 84	24, 37, 60, 94	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	266	ILE	4.4
1	J	264	SER	4.0
1	E	265	ALA	3.4
1	E	264	SER	3.2
1	I	158	ASP	3.1
1	G	254	PRO	3.1
1	I	162	GLY	2.7
1	H	158	ASP	2.3
1	D	160	LYS	2.3
1	I	256	PRO	2.3
1	I	261	GLU	2.3
1	I	257	LYS	2.2
1	D	158	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	267	LEU	2.1
1	G	256	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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.