



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:42 PM UTC

PDB ID : 5ZTE / pdb_00005zte
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

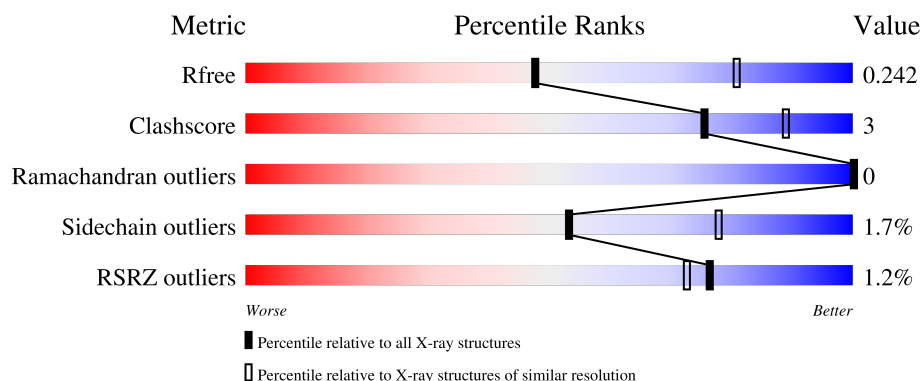
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	B	203	
1	C	203	
1	D	203	
1	E	203	

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Mol	Chain	Length	Quality of chain
1	F	203	94%
1	G	203	2% 87% 5% 8%
1	H	203	% 85% 10% 5%
1	I	203	% 88% 7%
1	J	203	% 82% 13%

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	O	0	0
			62	62		
2	B	58	Total	O	0	0
			58	58		
2	C	44	Total	O	0	0
			44	44		
2	D	32	Total	O	0	0
			32	32		
2	E	33	Total	O	0	0
			33	33		
2	F	83	Total	O	0	0
			83	83		
2	G	71	Total	O	0	0
			71	71		
2	H	36	Total	O	0	0
			36	36		
2	I	50	Total	O	0	0
			50	50		
2	J	41	Total	O	0	0
			41	41		

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: 2-Cys peroxiredoxin BAS1, chloroplastic

Chain A: 



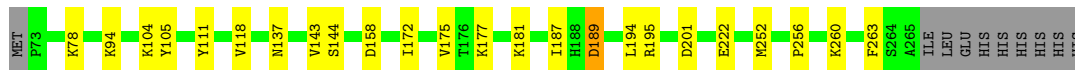
- Molecule 1: 2-Cys peroxiredoxin BAS1, chloroplastic

Chain B: 



- Molecule 1: 2-Cys peroxiredoxin BAS1, chloroplastic

Chain C: 



- Molecule 1: 2-Cys peroxiredoxin BAS1, chloroplastic

Chain D: 



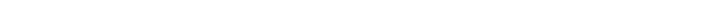
- Molecule 1: 2-Cys peroxiredoxin BAS1, chloroplastic

Chain E: 



- Molecule 1: 2-Cys peroxiredoxin BAS1, chloroplastic

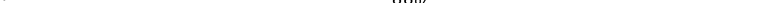
Diagram illustrating the structure of a protein, showing residues MET, P73, Y105, V118, V175, T176, K177, R195, D201, E268, and HIS. The residues are represented by colored blocks (grey, green, yellow) and connected by lines, indicating interactions or a sequence.

- Chain G:  2% 87% 5% 8%

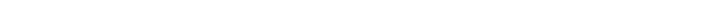
[illegible]

- Chain H:  %

[illegible]

- Chain I:  88% 7% .

[illegible]

- Chain J:  82% 13% 5%

Protein	Number of Mutations
MET	0
P73	10
K78	10
Y105	10
F109	10
D114	10
E122	10
M137	10
V143	10
D146	10
K160	15
L171	10
I172	10
S173	10
D174	10
V175	10
T176	10
K177	10
K181	15
L197	10
D201	10
K202	10
H208	10
S209	10
R218	10
E222	10
T226	10
Q231	10
M236	10
K246	10
M252	10
F263	15
S264	10
A265	10
T266	15
LEU	0
GLU	0

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 40.74 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.5 (40.74-2.60) 95.6 (40.74-2.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.61Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.196 , 0.244 0.195 , 0.242	Depositor DCC
R_{free} test set	3770 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtrriage
Anisotropy	0.012	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.27	0/1576	0.49	0/2133
1	B	0.27	0/1615	0.51	0/2183
1	C	0.26	0/1560	0.44	0/2111
1	D	0.25	0/1576	0.48	0/2133
1	E	0.24	0/1568	0.44	0/2122
1	F	0.27	0/1585	0.47	0/2145
1	G	0.27	0/1506	0.51	0/2039
1	H	0.26	0/1560	0.46	0/2111
1	I	0.25	0/1568	0.46	0/2122
1	J	0.24	0/1568	0.44	0/2122
All	All	0.26	0/15682	0.47	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	9	0
1	B	1575	0	1540	14	0
1	C	1524	0	1509	12	0
1	D	1540	0	1531	10	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	91	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 (91) 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	0.74
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:A:177:LYS:NZ	1:B:175:VAL:O	2.32	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:G:257:LYS:HG2	1:I:91:GLU:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	2.43	0.53
1:D:252:MET:HE1	1:D:263:PHE:CZ	2.45	0.51
1:J:122:GLU:CD	1:J:218:ARG:HH21	2.18	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:E:122:GLU:CD	1:E:218:ARG:HH21	2.20	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:137:ASN:HD22	1:H:202:LYS:HE3	1.77	0.49
1:H:173:SER:OG	1:H:175:VAL:HG23	2.13	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: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: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:I:252:MET:HE1	1:I:263:PHE:CE2	2.51	0.45
1:B:262:TYR:OH	1:D:85:GLU:OE2	2.30	0.45
1:D:230:LEU:O	1:D:234:GLN:HG3	2.17	0.45
1:J:105:TYR:CZ	1:J:231:GLN:HG2	2.52	0.45
1:B:103:LYS:HD3	1:H:237:PRO:HG3	1.96	0.45
1:C:252:MET:HE1	1:C:263:PHE:CE2	2.52	0.45
1:E:250:LYS:H	1:E:250:LYS:CE	2.30	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: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:D:122:GLU:CD	1:D:218:ARG:HH21	2.27	0.42
1:A:197:LEU:N	1:A:210:THR:O	2.44	0.42
1:B:122:GLU:CD	1:B:218:ARG:HH21	2.27	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:A:252:MET:HE1	1:A:263:PHE:CZ	2.55	0.42
1:I:252:MET:HE3	1:I:262:TYR:HB3	2.02	0.42
1:J:171:LEU:HD23	1:J:171:LEU:HA	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:252:MET:HE1	1:J:263:PHE:CE2	2.56	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:OD1	1:J:236:ASN:N	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%)	171 (99%)	1 (1%)	78	91
1	B	175/180 (97%)	171 (98%)	4 (2%)	44	71
1	C	170/180 (94%)	164 (96%)	6 (4%)	32	59
1	D	172/180 (96%)	171 (99%)	1 (1%)	78	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	171/180 (95%)	167 (98%)	4 (2%)	44	71
1	F	173/180 (96%)	173 (100%)	0	100	100
1	G	165/180 (92%)	162 (98%)	3 (2%)	51	76
1	H	170/180 (94%)	166 (98%)	4 (2%)	43	70
1	I	171/180 (95%)	168 (98%)	3 (2%)	51	76
1	J	171/180 (95%)	168 (98%)	3 (2%)	51	76
All	All	1710/1800 (95%)	1681 (98%)	29 (2%)	53	78

All (29) residues with a non-rotameric sidechain are listed below:

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	137	ASN
1	B	190	GLN
1	B	228	GLN
1	B	270	HIS
1	B	273	HIS
1	B	274	HIS
1	C	190	GLN
1	C	236	ASN
1	D	190	GLN
1	F	236	ASN
1	G	231	GLN
1	H	137	ASN
1	H	236	ASN
1	I	236	ASN
1	J	137	ASN
1	J	188	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 ⓘ

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%)	-0.37	1 (0%) 87 85	25, 33, 49, 58	0
1	B	198/203 (97%)	-0.06	7 (3%) 47 41	25, 35, 65, 94	0
1	C	193/203 (95%)	-0.24	0 100 100	25, 37, 57, 71	0
1	D	195/203 (96%)	-0.21	1 (0%) 87 85	27, 37, 61, 72	0
1	E	194/203 (95%)	-0.06	2 (1%) 79 76	30, 41, 63, 72	0
1	F	196/203 (96%)	-0.34	0 100 100	24, 32, 50, 75	0
1	G	187/203 (92%)	-0.18	5 (2%) 56 50	24, 33, 64, 94	0
1	H	193/203 (95%)	0.05	2 (1%) 79 76	28, 40, 60, 72	0
1	I	194/203 (95%)	-0.12	2 (1%) 79 76	28, 39, 64, 81	0
1	J	194/203 (95%)	-0.17	3 (1%) 72 68	28, 39, 63, 77	0
All	All	1939/2030 (95%)	-0.17	23 (1%) 76 73	24, 37, 60, 94	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	254	PRO	5.4
1	I	266	ILE	5.3
1	E	266	ILE	4.4
1	B	273	HIS	3.9
1	H	265	ALA	3.9
1	B	263	PHE	3.3
1	B	269	HIS	3.3
1	G	258	LEU	3.1
1	D	267	LEU	3.0
1	I	265	ALA	2.8
1	B	270	HIS	2.8
1	G	256	PRO	2.7
1	J	266	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	189	ASP	2.5
1	E	257	LYS	2.5
1	G	255	ASP	2.5
1	B	262	TYR	2.3
1	G	259	SER	2.3
1	B	272	HIS	2.2
1	J	160	LYS	2.2
1	A	267	LEU	2.1
1	J	264	SER	2.0
1	B	260	LYS	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 oligosaccharides 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.