



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:53 PM UTC

PDB ID : 2PRR / pdb_00002pr
Title : Crystal structure of alkylhydroperoxidase AhpD core: uncharacterized peroxidase-related protein (YP_296737.1) from *Ralstonia eutropha* JMP134 at 2.15 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2007-05-04
Resolution : 2.15 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:

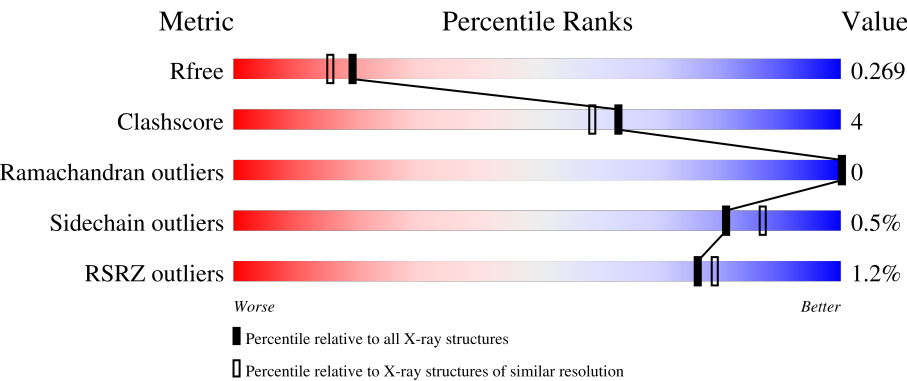
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	197	83%11% . .
1	B	197	2% 85%9% . .
1	C	197	% 87%7% . .
1	D	197	% 88%7% . .
1	E	197	% 87%9% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	197	81%13%
1	G	197	% 87%8%
1	H	197	% 86%9%
1	I	197	% 86%9%
1	J	197	2% 82%13%5%
1	K	197	2% 88%9%
1	L	197	2% 86%10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19292 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 Alkylhydroperoxidase AhpD core: uncharacterized peroxidase-related protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	190	Total	C	N	O	S	Se	0	1	0
			1497	960	260	268	3	6			
1	B	190	Total	C	N	O	S	Se	0	1	0
			1493	955	259	270	3	6			
1	C	189	Total	C	N	O	S	Se	0	0	0
			1483	951	257	266	3	6			
1	D	191	Total	C	N	O	S	Se	0	0	0
			1481	954	257	261	3	6			
1	E	190	Total	C	N	O	S	Se	0	0	0
			1486	952	260	265	3	6			
1	F	190	Total	C	N	O	S	Se	0	0	0
			1478	949	257	263	3	6			
1	G	189	Total	C	N	O	S	Se	0	0	0
			1474	945	256	264	3	6			
1	H	190	Total	C	N	O	S	Se	0	0	0
			1475	948	258	260	3	6			
1	I	189	Total	C	N	O	S	Se	0	0	0
			1462	935	255	263	3	6			
1	J	188	Total	C	N	O	S	Se	0	0	0
			1455	932	253	261	3	6			
1	K	191	Total	C	N	O	S	Se	0	0	0
			1463	937	257	260	3	6			
1	L	189	Total	C	N	O	S	Se	0	0	0
			1462	940	253	260	3	6			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q46Y90
A	1	MSE	MET	modified residue	UNP Q46Y90
A	62	MSE	MET	modified residue	UNP Q46Y90
A	75	MSE	MET	modified residue	UNP Q46Y90

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	126	MSE	MET	modified residue	UNP Q46Y90
A	174	MSE	MET	modified residue	UNP Q46Y90
A	180	MSE	MET	modified residue	UNP Q46Y90
A	189	MSE	MET	modified residue	UNP Q46Y90
B	0	GLY	-	expression tag	UNP Q46Y90
B	1	MSE	MET	modified residue	UNP Q46Y90
B	62	MSE	MET	modified residue	UNP Q46Y90
B	75	MSE	MET	modified residue	UNP Q46Y90
B	126	MSE	MET	modified residue	UNP Q46Y90
B	174	MSE	MET	modified residue	UNP Q46Y90
B	180	MSE	MET	modified residue	UNP Q46Y90
B	189	MSE	MET	modified residue	UNP Q46Y90
C	0	GLY	-	expression tag	UNP Q46Y90
C	1	MSE	MET	modified residue	UNP Q46Y90
C	62	MSE	MET	modified residue	UNP Q46Y90
C	75	MSE	MET	modified residue	UNP Q46Y90
C	126	MSE	MET	modified residue	UNP Q46Y90
C	174	MSE	MET	modified residue	UNP Q46Y90
C	180	MSE	MET	modified residue	UNP Q46Y90
C	189	MSE	MET	modified residue	UNP Q46Y90
D	0	GLY	-	expression tag	UNP Q46Y90
D	1	MSE	MET	modified residue	UNP Q46Y90
D	62	MSE	MET	modified residue	UNP Q46Y90
D	75	MSE	MET	modified residue	UNP Q46Y90
D	126	MSE	MET	modified residue	UNP Q46Y90
D	174	MSE	MET	modified residue	UNP Q46Y90
D	180	MSE	MET	modified residue	UNP Q46Y90
D	189	MSE	MET	modified residue	UNP Q46Y90
E	0	GLY	-	expression tag	UNP Q46Y90
E	1	MSE	MET	modified residue	UNP Q46Y90
E	62	MSE	MET	modified residue	UNP Q46Y90
E	75	MSE	MET	modified residue	UNP Q46Y90
E	126	MSE	MET	modified residue	UNP Q46Y90
E	174	MSE	MET	modified residue	UNP Q46Y90
E	180	MSE	MET	modified residue	UNP Q46Y90
E	189	MSE	MET	modified residue	UNP Q46Y90
F	0	GLY	-	expression tag	UNP Q46Y90
F	1	MSE	MET	modified residue	UNP Q46Y90
F	62	MSE	MET	modified residue	UNP Q46Y90
F	75	MSE	MET	modified residue	UNP Q46Y90
F	126	MSE	MET	modified residue	UNP Q46Y90
F	174	MSE	MET	modified residue	UNP Q46Y90

Continued on next page...

Continued from previous page...

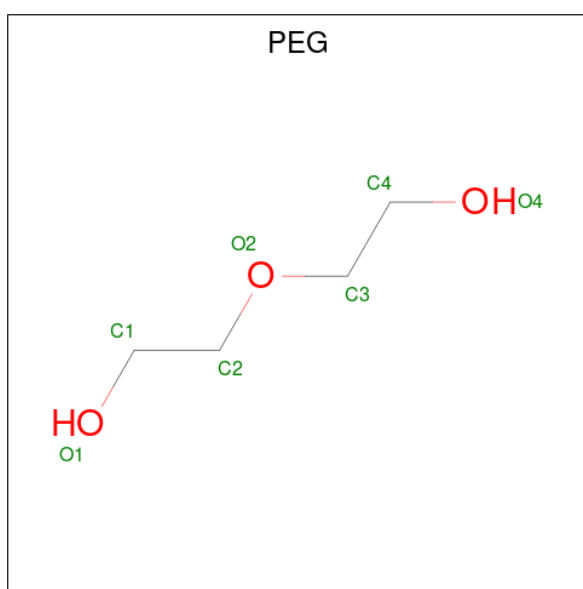
Chain	Residue	Modelled	Actual	Comment	Reference
F	180	MSE	MET	modified residue	UNP Q46Y90
F	189	MSE	MET	modified residue	UNP Q46Y90
G	0	GLY	-	expression tag	UNP Q46Y90
G	1	MSE	MET	modified residue	UNP Q46Y90
G	62	MSE	MET	modified residue	UNP Q46Y90
G	75	MSE	MET	modified residue	UNP Q46Y90
G	126	MSE	MET	modified residue	UNP Q46Y90
G	174	MSE	MET	modified residue	UNP Q46Y90
G	180	MSE	MET	modified residue	UNP Q46Y90
G	189	MSE	MET	modified residue	UNP Q46Y90
H	0	GLY	-	expression tag	UNP Q46Y90
H	1	MSE	MET	modified residue	UNP Q46Y90
H	62	MSE	MET	modified residue	UNP Q46Y90
H	75	MSE	MET	modified residue	UNP Q46Y90
H	126	MSE	MET	modified residue	UNP Q46Y90
H	174	MSE	MET	modified residue	UNP Q46Y90
H	180	MSE	MET	modified residue	UNP Q46Y90
H	189	MSE	MET	modified residue	UNP Q46Y90
I	0	GLY	-	expression tag	UNP Q46Y90
I	1	MSE	MET	modified residue	UNP Q46Y90
I	62	MSE	MET	modified residue	UNP Q46Y90
I	75	MSE	MET	modified residue	UNP Q46Y90
I	126	MSE	MET	modified residue	UNP Q46Y90
I	174	MSE	MET	modified residue	UNP Q46Y90
I	180	MSE	MET	modified residue	UNP Q46Y90
I	189	MSE	MET	modified residue	UNP Q46Y90
J	0	GLY	-	expression tag	UNP Q46Y90
J	1	MSE	MET	modified residue	UNP Q46Y90
J	62	MSE	MET	modified residue	UNP Q46Y90
J	75	MSE	MET	modified residue	UNP Q46Y90
J	126	MSE	MET	modified residue	UNP Q46Y90
J	174	MSE	MET	modified residue	UNP Q46Y90
J	180	MSE	MET	modified residue	UNP Q46Y90
J	189	MSE	MET	modified residue	UNP Q46Y90
K	0	GLY	-	expression tag	UNP Q46Y90
K	1	MSE	MET	modified residue	UNP Q46Y90
K	62	MSE	MET	modified residue	UNP Q46Y90
K	75	MSE	MET	modified residue	UNP Q46Y90
K	126	MSE	MET	modified residue	UNP Q46Y90
K	174	MSE	MET	modified residue	UNP Q46Y90
K	180	MSE	MET	modified residue	UNP Q46Y90
K	189	MSE	MET	modified residue	UNP Q46Y90

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	0	GLY	-	expression tag	UNP Q46Y90
L	1	MSE	MET	modified residue	UNP Q46Y90
L	62	MSE	MET	modified residue	UNP Q46Y90
L	75	MSE	MET	modified residue	UNP Q46Y90
L	126	MSE	MET	modified residue	UNP Q46Y90
L	174	MSE	MET	modified residue	UNP Q46Y90
L	180	MSE	MET	modified residue	UNP Q46Y90
L	189	MSE	MET	modified residue	UNP Q46Y90

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



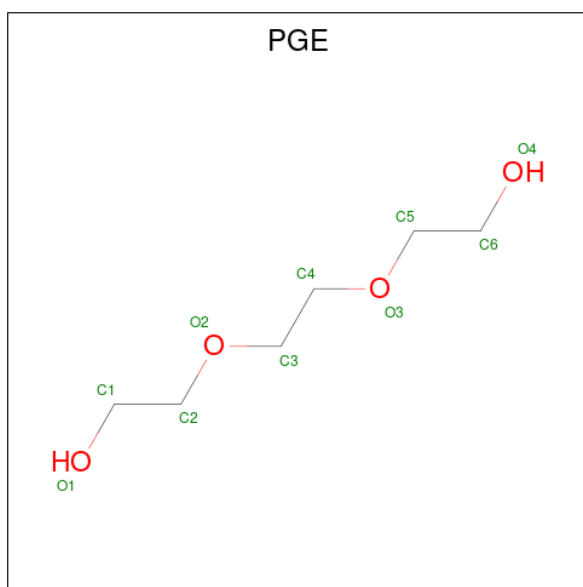
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 7 4 3	0	0
2	A	1	Total C O 7 4 3	0	0
2	A	1	Total C O 7 4 3	0	0
2	B	1	Total C O 7 4 3	0	0
2	B	1	Total C O 7 4 3	0	0
2	C	1	Total C O 7 4 3	0	0
2	C	1	Total C O 7 4 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			7	4	3		
2	D	1	Total	C	O	0	0
			7	4	3		
2	E	1	Total	C	O	0	0
			7	4	3		
2	E	1	Total	C	O	0	0
			7	4	3		
2	E	1	Total	C	O	0	0
			7	4	3		
2	F	1	Total	C	O	0	0
			7	4	3		
2	F	1	Total	C	O	0	0
			7	4	3		
2	G	1	Total	C	O	0	0
			7	4	3		
2	G	1	Total	C	O	0	0
			7	4	3		
2	H	1	Total	C	O	0	0
			7	4	3		
2	H	1	Total	C	O	0	0
			7	4	3		
2	I	1	Total	C	O	0	0
			7	4	3		
2	J	1	Total	C	O	0	0
			7	4	3		
2	J	1	Total	C	O	0	0
			7	4	3		
2	J	1	Total	C	O	0	0
			7	4	3		
2	K	1	Total	C	O	0	0
			7	4	3		
2	K	1	Total	C	O	0	0
			7	4	3		
2	L	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			10	6	4		
3	C	1	Total	C	O	0	0
			10	6	4		
3	D	1	Total	C	O	0	0
			10	6	4		
3	E	1	Total	C	O	0	0
			10	6	4		
3	F	1	Total	C	O	0	0
			10	6	4		
3	G	1	Total	C	O	0	0
			10	6	4		
3	H	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	133	Total	O	0	0
			133	133		
4	B	133	Total	O	0	0
			133	133		
4	C	122	Total	O	0	0
			122	122		
4	D	117	Total	O	0	0
			117	117		
4	E	130	Total	O	0	0
			130	130		

Continued on next page...

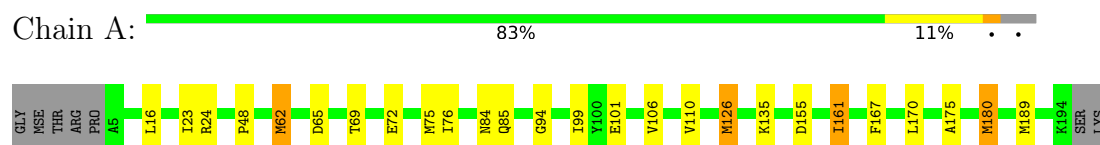
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	116	Total 116	O 116	0	0
4	G	102	Total 102	O 102	0	0
4	H	130	Total 130	O 130	0	0
4	I	107	Total 107	O 107	0	0
4	J	81	Total 81	O 81	0	0
4	K	88	Total 88	O 88	0	0
4	L	79	Total 79	O 79	0	0

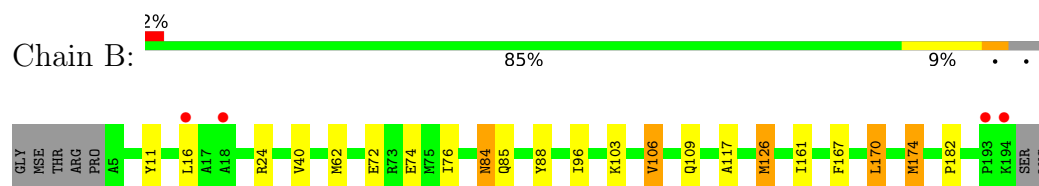
3 Residue-property plots [i](#)

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.

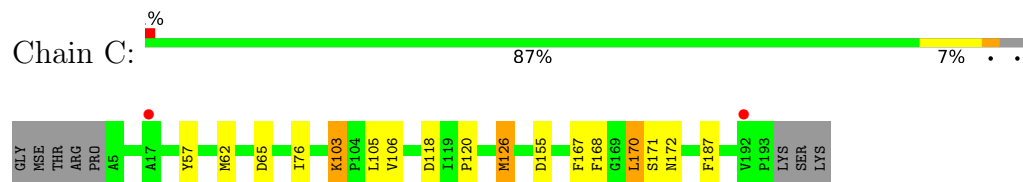
- Molecule 1: Alkylhydroperoxidase AhpD core: uncharacterized peroxidase-related protein



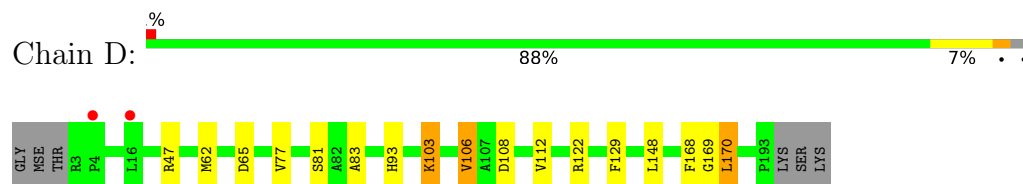
- Molecule 1: Alkylhydroperoxidase AhpD core: uncharacterized peroxidase-related protein



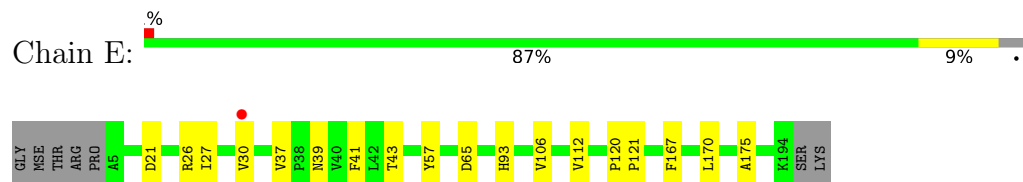
- Molecule 1: Alkylhydroperoxidase AhpD core: uncharacterized peroxidase-related protein



- Molecule 1: Alkylhydroperoxidase AhpD core: uncharacterized peroxidase-related protein

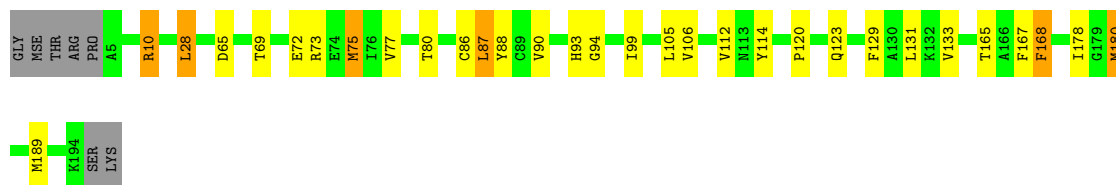


- Molecule 1: Alkylhydroperoxidase AhpD core: uncharacterized peroxidase-related protein



- Molecule 1: Alkylhydroperoxidase AhpD core: uncharacterized peroxidase-related protein

Chain F:  81% 13% . .



- Molecule 1: Alkylhydroperoxidase AhpD core: uncharacterized peroxidase-related protein

Chain G:  87% 8% . .



- Molecule 1: Alkylhydroperoxidase AhpD core: uncharacterized peroxidase-related protein

Chain H:  86% 9% . .



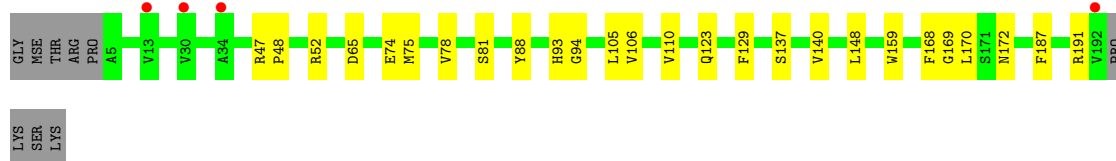
- Molecule 1: Alkylhydroperoxidase AhpD core: uncharacterized peroxidase-related protein

Chain I:  86% 9% . .



- Molecule 1: Alkylhydroperoxidase AhpD core: uncharacterized peroxidase-related protein

Chain J:  82% 13% 5%

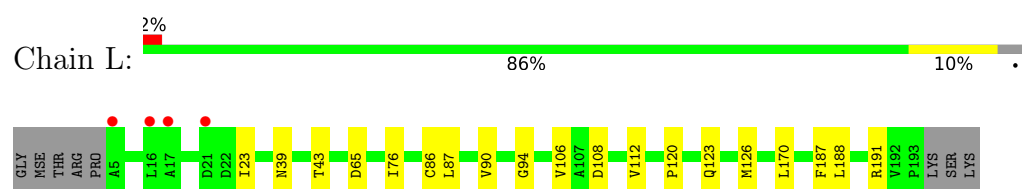


- Molecule 1: Alkylhydroperoxidase AhpD core: uncharacterized peroxidase-related protein

Chain K:  88% 9% .



- Molecule 1: Alkylhydroperoxidase AhpD core: uncharacterized peroxidase-related protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.11Å 93.95Å 120.90Å 84.26° 81.64° 77.73°	Depositor
Resolution (Å)	48.91 – 2.15 48.91 – 2.15	Depositor EDS
% Data completeness (in resolution range)	94.7 (48.91-2.15) 94.5 (48.91-2.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.211 , 0.262 0.220 , 0.269	Depositor DCC
R_{free} test set	7717 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19292	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	1.10	4/1526 (0.3%)	1.09	3/2060 (0.1%)
1	B	1.07	5/1522 (0.3%)	1.09	1/2057 (0.0%)
1	C	0.97	2/1512 (0.1%)	1.10	8/2041 (0.4%)
1	D	1.01	3/1511 (0.2%)	1.08	7/2042 (0.3%)
1	E	0.91	0/1515	1.07	5/2046 (0.2%)
1	F	0.98	3/1507 (0.2%)	1.12	4/2036 (0.2%)
1	G	0.93	1/1503 (0.1%)	1.05	5/2030 (0.2%)
1	H	1.00	3/1504 (0.2%)	1.08	1/2032 (0.0%)
1	I	0.99	2/1491 (0.1%)	1.08	6/2015 (0.3%)
1	J	0.90	1/1483 (0.1%)	1.09	6/2002 (0.3%)
1	K	0.92	2/1493 (0.1%)	1.05	4/2020 (0.2%)
1	L	0.87	0/1491	1.07	4/2015 (0.2%)
All	All	0.97	26/18058 (0.1%)	1.08	54/24396 (0.2%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	MSE	SE-CE	17.50	2.48	1.95
1	C	126	MSE	SE-CE	13.04	2.34	1.95
1	F	180	MSE	SE-CE	12.55	2.33	1.95
1	B	174	MSE	SE-CE	12.09	2.31	1.95
1	H	126	MSE	SE-CE	11.79	2.30	1.95
1	A	62	MSE	SE-CE	11.52	2.30	1.95
1	D	62	MSE	SE-CE	-11.40	1.61	1.95
1	H	180	MSE	SE-CE	10.04	2.25	1.95
1	I	126	MSE	SE-CE	-9.56	1.66	1.95
1	B	126	MSE	SE-CE	-9.48	1.67	1.95
1	G	62	MSE	SE-CE	-8.82	1.69	1.95
1	F	75	MSE	SE-CE	-8.09	1.71	1.95
1	I	126	MSE	CG-SE	7.96	2.19	1.95
1	H	75	MSE	SE-CE	-7.26	1.73	1.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	180	MSE	SE-CE	-6.97	1.74	1.95
1	A	180	MSE	SE-CE	6.89	2.16	1.95
1	D	168	PHE	C-O	-6.33	1.15	1.24
1	B	84	ASN	CA-C	5.71	1.60	1.52
1	K	88	TYR	C-O	-5.60	1.17	1.24
1	F	168	PHE	C-O	-5.59	1.16	1.24
1	J	168	PHE	C-O	-5.54	1.16	1.24
1	D	83	ALA	N-CA	5.45	1.53	1.46
1	B	62	MSE	SE-CE	5.43	2.11	1.95
1	C	62	MSE	SE-CE	5.33	2.11	1.95
1	A	161	ILE	CA-CB	5.17	1.60	1.54
1	B	126	MSE	CG-SE	5.13	2.10	1.95

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	106	VAL	N-CA-C	8.49	119.28	110.62
1	E	106	VAL	N-CA-C	7.33	118.09	110.62
1	J	169	GLY	N-CA-C	-7.25	104.09	112.50
1	L	65	ASP	N-CA-C	-6.59	99.79	110.20
1	F	94	GLY	N-CA-C	-6.55	104.87	112.73
1	L	94	GLY	N-CA-C	-6.47	104.48	112.77
1	J	65	ASP	N-CA-C	-6.34	100.45	109.96
1	G	94	GLY	N-CA-C	-6.15	105.05	112.49
1	H	106	VAL	N-CA-C	6.14	116.88	110.62
1	G	89	CYS	N-CA-C	6.07	117.98	111.36
1	K	106	VAL	N-CA-C	5.94	118.48	111.05
1	A	65	ASP	N-CA-C	-5.84	100.98	110.20
1	A	126	MSE	CG-SE-CE	5.80	111.68	98.92
1	I	77	VAL	CB-CA-C	-5.80	104.42	112.02
1	C	106	VAL	N-CA-C	5.78	116.51	110.62
1	D	169	GLY	N-CA-C	-5.76	105.65	113.37
1	G	106	VAL	N-CA-C	5.73	119.08	111.17
1	D	106	VAL	N-CA-C	5.72	116.45	110.62
1	D	65	ASP	N-CA-C	-5.69	101.20	110.20
1	J	94	GLY	N-CA-C	-5.64	105.96	112.50
1	A	94	GLY	N-CA-C	-5.63	105.97	112.73
1	L	106	VAL	N-CA-C	5.63	116.36	110.62
1	C	76	ILE	CB-CA-C	-5.62	104.55	112.14
1	C	65	ASP	N-CA-C	-5.49	101.03	109.76
1	I	94	GLY	N-CA-C	-5.48	105.75	112.77
1	B	106	VAL	N-CA-C	5.48	117.94	111.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	65	ASP	N-CA-C	-5.45	101.58	110.20
1	C	103	LYS	CA-C-N	5.43	125.10	119.56
1	C	103	LYS	C-N-CA	5.43	125.10	119.56
1	F	65	ASP	N-CA-C	-5.42	101.63	110.20
1	I	65	ASP	N-CA-C	-5.41	101.17	109.76
1	G	19	LEU	N-CA-C	5.33	117.32	110.39
1	J	47	ARG	CA-C-N	5.30	125.36	119.32
1	J	47	ARG	C-N-CA	5.30	125.36	119.32
1	J	168	PHE	N-CA-C	5.27	118.97	112.54
1	C	172	ASN	CB-CA-C	-5.23	101.97	110.85
1	I	103	LYS	CA-C-N	5.22	124.89	119.56
1	I	103	LYS	C-N-CA	5.22	124.89	119.56
1	K	170	LEU	N-CA-C	-5.21	105.25	111.03
1	F	87	LEU	N-CA-C	5.18	116.61	111.07
1	K	120	PRO	CA-C-N	5.17	125.21	119.32
1	K	120	PRO	C-N-CA	5.17	125.21	119.32
1	E	120	PRO	CA-C-N	5.12	126.24	119.84
1	E	120	PRO	C-N-CA	5.12	126.24	119.84
1	D	47	ARG	CA-C-N	5.12	126.24	119.84
1	D	47	ARG	C-N-CA	5.12	126.24	119.84
1	C	120	PRO	CA-C-N	5.12	125.16	119.32
1	C	120	PRO	C-N-CA	5.12	125.16	119.32
1	G	172	ASN	N-CA-C	5.10	116.84	111.28
1	L	23	ILE	N-CA-C	-5.08	105.90	110.82
1	D	103	LYS	CA-C-N	5.07	124.73	119.56
1	D	103	LYS	C-N-CA	5.07	124.73	119.56
1	I	106	VAL	N-CA-C	5.06	115.78	110.62
1	E	21	ASP	N-CA-C	5.05	116.48	111.07

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	1497	0	1475	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1493	0	1450	19	0
1	C	1483	0	1458	8	0
1	D	1481	0	1450	7	0
1	E	1486	0	1459	11	0
1	F	1478	0	1445	24	0
1	G	1474	0	1438	11	0
1	H	1475	0	1444	14	0
1	I	1462	0	1410	11	0
1	J	1455	0	1406	16	0
1	K	1463	0	1405	7	0
1	L	1462	0	1423	10	0
2	A	21	0	30	0	0
2	B	14	0	20	1	0
2	C	21	0	30	0	0
2	D	7	0	10	1	0
2	E	21	0	30	4	0
2	F	14	0	20	1	0
2	G	14	0	20	0	0
2	H	14	0	20	1	0
2	I	7	0	10	0	0
2	J	21	0	30	1	0
2	K	14	0	20	0	0
2	L	7	0	10	0	0
3	B	10	0	14	0	0
3	C	10	0	14	0	0
3	D	10	0	14	0	0
3	E	10	0	14	0	0
3	F	10	0	14	2	0
3	G	10	0	14	0	0
3	H	10	0	14	0	0
4	A	133	0	0	1	0
4	B	133	0	0	0	0
4	C	122	0	0	0	0
4	D	117	0	0	1	0
4	E	130	0	0	1	0
4	F	116	0	0	0	0
4	G	102	0	0	0	0
4	H	130	0	0	0	0
4	I	107	0	0	2	0
4	J	81	0	0	0	0
4	K	88	0	0	0	0
4	L	79	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	19292	0	17611	141	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 4.

All (141) 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:A:180:MSE:CE	1:A:180:MSE:SE	2.16	1.43
1:I:126:MSE:SE	1:I:126:MSE:CG	2.19	1.41
1:H:180:MSE:SE	1:H:180:MSE:CE	2.25	1.34
1:H:126:MSE:SE	1:H:126:MSE:CE	2.30	1.29
1:A:62:MSE:CE	1:A:62:MSE:SE	2.30	1.28
1:B:174:MSE:SE	1:B:174:MSE:CE	2.31	1.28
1:F:180:MSE:SE	1:F:180:MSE:CE	2.33	1.27
1:C:126:MSE:CE	1:C:126:MSE:SE	2.34	1.25
1:A:126:MSE:SE	1:A:126:MSE:CE	2.48	1.12
1:B:174:MSE:CE	1:B:174:MSE:HB3	2.20	0.70
1:G:103:LYS:NZ	1:G:118:ASP:O	2.27	0.68
1:F:178:ILE:HD11	1:F:180:MSE:HE3	1.77	0.65
1:H:170:LEU:C	1:H:170:LEU:HD23	2.22	0.65
1:E:112:VAL:HG11	1:H:87:LEU:HA	1.80	0.63
1:H:93:HIS:NE2	2:H:199:PEG:H12	2.15	0.62
1:I:46:HIS:ND1	4:I:229:HOH:O	2.31	0.62
1:K:16:LEU:O	1:K:24:ARG:HD3	2.00	0.62
1:B:40:VAL:HG11	2:B:198:PEG:H32	1.81	0.61
1:D:108:ASP:O	1:D:112:VAL:HG23	2.00	0.60
1:F:77:VAL:HG22	1:F:168:PHE:CD2	2.36	0.60
1:G:62:MSE:HE2	1:G:62:MSE:HA	1.84	0.59
1:B:174:MSE:HB3	1:B:174:MSE:HE3	1.83	0.58
1:E:93:HIS:NE2	2:E:199:PEG:C1	2.67	0.58
1:A:99[B]:ILE:HD11	1:A:189:MSE:HG2	1.85	0.58
1:L:86:CYS:O	1:L:90:VAL:HG23	2.04	0.57
1:F:87:LEU:HA	1:L:112:VAL:HG11	1.88	0.56
1:I:126:MSE:SE	1:I:126:MSE:CB	3.00	0.56
1:A:167:PHE:HA	1:B:170:LEU:HD12	1.87	0.55
1:E:170:LEU:C	1:E:170:LEU:HD23	2.31	0.55
1:H:43:THR:OG1	1:H:180:MSE:HE2	2.07	0.55
1:A:16:LEU:HD22	1:A:24:ARG:HG3	1.89	0.55
1:B:103:LYS:O	1:B:106:VAL:HG12	2.07	0.55
1:B:170:LEU:C	1:B:170:LEU:HD23	2.32	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:93:HIS:NE2	2:E:199:PEG:H12	2.22	0.54
1:F:86:CYS:O	1:F:90:VAL:HG23	2.07	0.54
1:F:178:ILE:HD11	1:F:180:MSE:CE	2.38	0.54
1:A:75:MSE:SE	1:A:126:MSE:CE	3.06	0.53
1:B:16:LEU:HB2	1:B:24:ARG:HG3	1.90	0.53
1:B:72:GLU:HB3	1:B:126:MSE:SE	2.59	0.53
1:C:103:LYS:NZ	1:C:118:ASP:O	2.38	0.52
1:F:93:HIS:NE2	2:F:199:PEG:H41	2.25	0.52
1:J:187:PHE:O	1:J:191:ARG:NH1	2.42	0.52
1:B:174:MSE:CE	1:B:174:MSE:CB	2.86	0.52
1:E:26:ARG:O	1:E:30:VAL:HG23	2.10	0.52
1:L:76:ILE:HG13	1:L:126:MSE:HE3	1.92	0.52
1:G:187:PHE:CD1	1:J:105:LEU:HD22	2.45	0.51
1:B:126:MSE:HG3	1:B:161:ILE:HD11	1.91	0.51
1:F:112:VAL:HG11	1:L:87:LEU:HA	1.93	0.51
1:J:74:GLU:O	1:J:78:VAL:HG23	2.11	0.51
1:F:105:LEU:HD22	1:L:187:PHE:CD1	2.46	0.50
1:L:170:LEU:C	1:L:170:LEU:HD23	2.36	0.50
1:H:114:TYR:CE1	1:H:131:LEU:CD1	2.95	0.50
1:E:57:TYR:HB3	1:E:167:PHE:CE1	2.47	0.49
1:J:75:MSE:HE1	1:J:123:GLN:OE1	2.12	0.49
1:F:99:ILE:HD11	1:F:189:MSE:HG2	1.95	0.49
1:F:167:PHE:HA	1:J:170:LEU:HD12	1.95	0.49
1:J:48:PRO:O	1:J:52:ARG:HG3	2.14	0.48
1:K:127:LEU:O	1:K:131:LEU:HD23	2.13	0.48
1:C:105:LEU:HD22	1:K:187:PHE:CG	2.49	0.48
1:D:93:HIS:NE2	2:D:198:PEG:H31	2.28	0.48
1:D:170:LEU:C	1:D:170:LEU:HD23	2.38	0.48
1:A:84:ASN:O	1:A:85:GLN:C	2.54	0.48
1:I:74:GLU:O	1:I:78:VAL:HG23	2.14	0.48
1:J:93:HIS:NE2	2:J:199:PEG:H41	2.28	0.48
1:E:93:HIS:NE2	2:E:199:PEG:H11	2.29	0.48
1:G:188:LEU:O	1:G:188:LEU:HD23	2.13	0.48
1:H:80:THR:HG21	1:H:165:THR:HG23	1.95	0.48
1:D:122:ARG:NE	4:D:298:HOH:O	2.42	0.48
1:F:88:TYR:C	1:F:88:TYR:CD1	2.92	0.47
1:A:170:LEU:C	1:A:170:LEU:HD23	2.39	0.47
1:E:39:ASN:O	1:E:43:THR:HG23	2.13	0.47
1:F:80:THR:HG21	1:F:165:THR:HG23	1.96	0.47
3:F:197:PGE:H1	1:L:108:ASP:OD1	2.14	0.47
1:J:137:SER:HA	1:J:140:VAL:HG23	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:170:LEU:C	1:J:170:LEU:HD23	2.40	0.46
1:A:69:THR:OG1	1:A:72:GLU:HG3	2.16	0.46
1:I:43:THR:OG1	1:I:180:MSE:HE2	2.16	0.46
1:I:135:LYS:NZ	4:I:299:HOH:O	2.48	0.46
1:G:170:LEU:C	1:G:170:LEU:HD23	2.41	0.46
1:F:72:GLU:CG	1:F:123:GLN:HE21	2.28	0.46
1:F:114:TYR:CE1	1:F:131:LEU:HD13	2.51	0.45
1:H:16:LEU:HD22	1:H:24:ARG:HG3	1.97	0.45
1:F:69:THR:O	1:F:73:ARG:HG3	2.16	0.45
1:F:72:GLU:HG2	1:F:123:GLN:HE21	1.81	0.45
1:J:88:TYR:C	1:J:88:TYR:CD1	2.94	0.45
1:I:126:MSE:CG	1:I:126:MSE:CE	2.91	0.45
1:G:187:PHE:CG	1:J:105:LEU:HD22	2.52	0.45
1:J:74:GLU:OE1	1:J:93:HIS:ND1	2.43	0.45
1:A:84:ASN:OD1	1:A:135:LYS:NZ	2.47	0.45
1:H:167:PHE:HA	1:I:170:LEU:HD12	1.98	0.45
1:A:23:ILE:CD1	1:A:48:PRO:HB3	2.45	0.45
1:D:103:LYS:O	1:D:106:VAL:HG12	2.17	0.45
1:B:109:GLN:HB3	1:B:117:ALA:HA	1.99	0.45
1:D:77:VAL:O	1:D:81:SER:OG	2.16	0.45
1:F:10:ARG:HG2	1:F:10:ARG:HH11	1.82	0.45
1:L:39:ASN:O	1:L:43:THR:HG23	2.16	0.45
1:A:175:ALA:HA	1:A:180:MSE:HB2	1.99	0.44
1:A:76:ILE:HD13	1:A:161:ILE:HG23	1.99	0.44
1:H:16:LEU:HD21	1:H:27:ILE:HG21	1.98	0.44
1:A:106:VAL:O	1:A:110:VAL:HG23	2.17	0.44
1:C:168:PHE:HA	1:C:171:SER:HB3	1.99	0.44
1:J:81:SER:HA	1:J:172:ASN:OD1	2.18	0.44
1:B:88:TYR:CD1	1:B:182:PRO:HA	2.52	0.44
1:J:106:VAL:O	1:J:110:VAL:HG23	2.18	0.44
1:A:170:LEU:HD12	1:B:167:PHE:HA	2.00	0.43
1:B:76:ILE:CG1	1:B:126:MSE:HE3	2.48	0.43
1:C:167:PHE:HA	1:G:170:LEU:HD12	1.99	0.43
1:F:120:PRO:HD2	1:F:123:GLN:OE1	2.18	0.42
1:B:84:ASN:O	1:B:85:GLN:C	2.60	0.42
1:K:132:LYS:NZ	1:K:144:ASP:OD2	2.49	0.42
1:C:155:ASP:O	1:G:11:TYR:OH	2.35	0.42
1:E:175:ALA:HB1	4:E:256:HOH:O	2.18	0.42
2:E:200:PEG:O1	1:H:179:GLY:O	2.29	0.42
1:K:95:ALA:O	1:K:99:ILE:HG12	2.20	0.42
1:L:120:PRO:HD2	1:L:123:GLN:OE1	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:129:PHE:O	1:F:133:VAL:HG23	2.20	0.42
1:C:170:LEU:C	1:C:170:LEU:HD23	2.45	0.42
1:J:129:PHE:CD2	1:J:148:LEU:HD11	2.54	0.42
1:F:28:LEU:C	1:F:28:LEU:HD12	2.45	0.42
1:G:160:ASP:O	1:G:164:ILE:HG13	2.20	0.42
1:C:187:PHE:CD1	1:K:105:LEU:HD22	2.55	0.42
1:B:88:TYR:CE1	1:B:182:PRO:HA	2.55	0.41
1:E:30:VAL:HG21	1:E:41:PHE:CZ	2.55	0.41
1:A:101:GLU:OE2	4:A:241:HOH:O	2.21	0.41
1:F:75:MSE:HE3	1:F:75:MSE:HB2	1.94	0.41
1:K:74:GLU:O	1:K:78:VAL:HG23	2.20	0.41
1:B:74:GLU:HG3	1:B:96:ILE:HG22	2.01	0.41
1:D:129:PHE:CG	1:D:148:LEU:HD11	2.56	0.41
1:F:90:VAL:HG12	3:F:197:PGE:H5	2.01	0.41
1:H:44:LEU:HD21	1:H:180:MSE:CE	2.51	0.41
1:A:155:ASP:O	1:B:11:TYR:OH	2.37	0.41
1:H:14:PRO:CG	1:H:19:LEU:HD21	2.51	0.41
1:I:26:ARG:NH2	1:I:55:PHE:HB3	2.36	0.41
1:I:109:GLN:HB3	1:I:117:ALA:HA	2.03	0.41
1:L:188:LEU:O	1:L:191:ARG:HG3	2.21	0.41
1:F:99:ILE:HD11	1:F:189:MSE:CG	2.51	0.41
1:G:192:VAL:O	1:G:192:VAL:HG13	2.21	0.40
1:I:99:ILE:HG13	1:I:189:MSE:HE3	2.02	0.40
1:E:27:ILE:HG23	1:E:37:VAL:HG11	2.03	0.40
1:G:16:LEU:HD21	1:G:27:ILE:HG21	2.03	0.40
1:J:159:TRP:C	1:J:159:TRP:CD1	2.99	0.40

There are no symmetry-related clashes.

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	189/197 (96%)	185 (98%)	4 (2%)	0	100	100
1	B	189/197 (96%)	185 (98%)	4 (2%)	0	100	100
1	C	187/197 (95%)	185 (99%)	2 (1%)	0	100	100
1	D	189/197 (96%)	184 (97%)	5 (3%)	0	100	100
1	E	188/197 (95%)	184 (98%)	4 (2%)	0	100	100
1	F	188/197 (95%)	186 (99%)	2 (1%)	0	100	100
1	G	187/197 (95%)	185 (99%)	2 (1%)	0	100	100
1	H	188/197 (95%)	184 (98%)	4 (2%)	0	100	100
1	I	187/197 (95%)	181 (97%)	6 (3%)	0	100	100
1	J	186/197 (94%)	183 (98%)	3 (2%)	0	100	100
1	K	189/197 (96%)	186 (98%)	3 (2%)	0	100	100
1	L	187/197 (95%)	182 (97%)	5 (3%)	0	100	100
All	All	2254/2364 (95%)	2210 (98%)	44 (2%)	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	152/154 (99%)	152 (100%)	0	100	100
1	B	150/154 (97%)	149 (99%)	1 (1%)	76	82
1	C	150/154 (97%)	148 (99%)	2 (1%)	61	68
1	D	146/154 (95%)	145 (99%)	1 (1%)	76	82
1	E	150/154 (97%)	149 (99%)	1 (1%)	76	82
1	F	147/154 (96%)	145 (99%)	2 (1%)	59	66
1	G	147/154 (96%)	146 (99%)	1 (1%)	76	82
1	H	146/154 (95%)	146 (100%)	0	100	100
1	I	144/154 (94%)	144 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	142/154 (92%)	142 (100%)	0	100	100
1	K	142/154 (92%)	142 (100%)	0	100	100
1	L	144/154 (94%)	144 (100%)	0	100	100
All	All	1760/1848 (95%)	1752 (100%)	8 (0%)	81	87

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	170	LEU
1	C	57	TYR
1	C	170	LEU
1	D	170	LEU
1	E	121	PRO
1	F	10	ARG
1	F	28	LEU
1	G	170	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	ASN
1	D	6	HIS
1	D	85	GLN
1	F	6	HIS
1	F	25	GLN
1	F	58	HIS
1	F	85	GLN
1	F	123	GLN
1	H	6	HIS
1	H	31	GLN
1	I	85	GLN
1	K	6	HIS
1	K	85	GLN
1	K	151	HIS
1	L	85	GLN

5.3.3 RNA ⓘ

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](#)

32 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PGE	H	197	-	9,9,9	0.49	0	8,8,8	0.64	0
2	PEG	K	197	-	6,6,6	0.43	0	5,5,5	0.34	0
2	PEG	G	199	-	6,6,6	0.57	0	5,5,5	0.63	0
2	PEG	J	199	-	6,6,6	0.45	0	5,5,5	0.73	0
2	PEG	C	198	-	6,6,6	0.69	0	5,5,5	0.56	0
2	PEG	A	199	-	6,6,6	0.58	0	5,5,5	0.30	0
2	PEG	D	198	-	6,6,6	0.59	0	5,5,5	0.61	0
2	PEG	F	198	-	6,6,6	0.58	0	5,5,5	0.22	0
2	PEG	J	197	-	6,6,6	0.45	0	5,5,5	0.62	0
3	PGE	D	197	-	9,9,9	0.50	0	8,8,8	0.30	0
3	PGE	G	197	-	9,9,9	0.40	0	8,8,8	0.34	0
2	PEG	E	199	-	6,6,6	0.39	0	5,5,5	0.73	0
2	PEG	A	197	-	6,6,6	0.38	0	5,5,5	0.22	0
3	PGE	B	197	-	9,9,9	0.47	0	8,8,8	0.34	0
2	PEG	E	200	-	6,6,6	0.47	0	5,5,5	0.33	0
3	PGE	E	197	-	9,9,9	0.31	0	8,8,8	0.61	0
3	PGE	C	197	-	9,9,9	0.45	0	8,8,8	0.45	0
2	PEG	C	200	-	6,6,6	0.53	0	5,5,5	0.42	0
2	PEG	H	199	-	6,6,6	0.54	0	5,5,5	0.77	0
2	PEG	G	198	-	6,6,6	0.52	0	5,5,5	0.21	0
2	PEG	B	199	-	6,6,6	0.47	0	5,5,5	0.50	0
2	PEG	I	197	-	6,6,6	0.61	0	5,5,5	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PEG	J	198	-	6,6,6	0.37	0	5,5,5	0.53	0
2	PEG	B	198	-	6,6,6	0.58	0	5,5,5	0.47	0
2	PEG	E	198	-	6,6,6	0.70	0	5,5,5	0.38	0
2	PEG	F	199	-	6,6,6	0.49	0	5,5,5	0.70	0
2	PEG	A	198	-	6,6,6	0.60	0	5,5,5	0.32	0
2	PEG	H	198	-	6,6,6	0.47	0	5,5,5	0.38	0
2	PEG	L	197	-	6,6,6	0.49	0	5,5,5	0.48	0
2	PEG	C	199	-	6,6,6	0.58	0	5,5,5	0.29	0
2	PEG	K	198	-	6,6,6	0.49	0	5,5,5	0.62	0
3	PGE	F	197	-	9,9,9	0.41	0	8,8,8	0.38	0

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
3	PGE	H	197	-	-	3/7/7/7	-
2	PEG	K	197	-	-	2/4/4/4	-
2	PEG	G	199	-	-	4/4/4/4	-
2	PEG	J	199	-	-	2/4/4/4	-
2	PEG	C	198	-	-	3/4/4/4	-
2	PEG	A	199	-	-	3/4/4/4	-
2	PEG	D	198	-	-	2/4/4/4	-
2	PEG	F	198	-	-	1/4/4/4	-
2	PEG	J	197	-	-	3/4/4/4	-
3	PGE	D	197	-	-	1/7/7/7	-
3	PGE	G	197	-	-	5/7/7/7	-
2	PEG	E	199	-	-	4/4/4/4	-
2	PEG	A	197	-	-	1/4/4/4	-
3	PGE	B	197	-	-	2/7/7/7	-
2	PEG	E	200	-	-	1/4/4/4	-
3	PGE	E	197	-	-	1/7/7/7	-
3	PGE	C	197	-	-	3/7/7/7	-
2	PEG	C	200	-	-	3/4/4/4	-
2	PEG	H	199	-	-	3/4/4/4	-
2	PEG	G	198	-	-	1/4/4/4	-
2	PEG	B	199	-	-	2/4/4/4	-
2	PEG	I	197	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	J	198	-	-	2/4/4/4	-
2	PEG	B	198	-	-	3/4/4/4	-
2	PEG	E	198	-	-	0/4/4/4	-
2	PEG	F	199	-	-	3/4/4/4	-
2	PEG	A	198	-	-	1/4/4/4	-
2	PEG	H	198	-	-	4/4/4/4	-
2	PEG	L	197	-	-	3/4/4/4	-
2	PEG	C	199	-	-	2/4/4/4	-
2	PEG	K	198	-	-	3/4/4/4	-
3	PGE	F	197	-	-	0/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	199	PEG	C4-C3-O2-C2
3	G	197	PGE	O2-C3-C4-O3
2	J	197	PEG	C1-C2-O2-C3
2	D	198	PEG	O1-C1-C2-O2
2	F	199	PEG	O1-C1-C2-O2
2	J	198	PEG	O1-C1-C2-O2
3	C	197	PGE	O3-C5-C6-O4
2	A	199	PEG	O2-C3-C4-O4
2	B	199	PEG	O1-C1-C2-O2
2	C	198	PEG	O1-C1-C2-O2
2	C	198	PEG	O2-C3-C4-O4
2	C	199	PEG	O1-C1-C2-O2
2	C	199	PEG	O2-C3-C4-O4
2	E	199	PEG	O1-C1-C2-O2
3	G	197	PGE	O3-C5-C6-O4
3	H	197	PGE	O1-C1-C2-O2
2	C	200	PEG	O1-C1-C2-O2
2	C	200	PEG	O2-C3-C4-O4
2	F	198	PEG	O2-C3-C4-O4
2	G	199	PEG	O1-C1-C2-O2
2	H	199	PEG	C1-C2-O2-C3
2	B	198	PEG	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	199	PEG	O2-C3-C4-O4
2	E	200	PEG	O2-C3-C4-O4
2	G	198	PEG	O2-C3-C4-O4
2	K	197	PEG	O1-C1-C2-O2
2	K	198	PEG	O1-C1-C2-O2
3	E	197	PGE	O3-C5-C6-O4
2	K	198	PEG	C1-C2-O2-C3
3	H	197	PGE	O2-C3-C4-O3
2	H	199	PEG	O2-C3-C4-O4
2	L	197	PEG	O1-C1-C2-O2
2	B	198	PEG	O2-C3-C4-O4
2	F	199	PEG	O2-C3-C4-O4
2	H	198	PEG	O2-C3-C4-O4
2	K	198	PEG	O2-C3-C4-O4
2	H	198	PEG	O1-C1-C2-O2
2	J	199	PEG	O2-C3-C4-O4
2	I	197	PEG	O1-C1-C2-O2
3	C	197	PGE	O2-C3-C4-O3
2	H	199	PEG	O1-C1-C2-O2
2	B	198	PEG	C1-C2-O2-C3
3	D	197	PGE	C1-C2-O2-C3
2	E	199	PEG	C4-C3-O2-C2
2	G	199	PEG	C1-C2-O2-C3
3	B	197	PGE	C6-C5-O3-C4
2	L	197	PEG	C4-C3-O2-C2
2	D	198	PEG	C4-C3-O2-C2
3	G	197	PGE	O1-C1-C2-O2
3	G	197	PGE	C3-C4-O3-C5
2	J	198	PEG	C4-C3-O2-C2
2	I	197	PEG	C1-C2-O2-C3
2	A	197	PEG	O2-C3-C4-O4
2	G	199	PEG	O2-C3-C4-O4
2	J	197	PEG	O1-C1-C2-O2
2	C	200	PEG	C4-C3-O2-C2
3	B	197	PGE	C1-C2-O2-C3
2	E	199	PEG	C1-C2-O2-C3
2	A	199	PEG	C1-C2-O2-C3
3	H	197	PGE	C1-C2-O2-C3
2	H	198	PEG	C1-C2-O2-C3
3	G	197	PGE	C4-C3-O2-C2
2	J	197	PEG	O2-C3-C4-O4
3	C	197	PGE	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	198	PEG	C1-C2-O2-C3
2	G	199	PEG	C4-C3-O2-C2
2	K	197	PEG	O2-C3-C4-O4
2	F	199	PEG	C4-C3-O2-C2
2	H	198	PEG	C4-C3-O2-C2
2	B	199	PEG	C1-C2-O2-C3
2	A	199	PEG	O1-C1-C2-O2
2	L	197	PEG	C1-C2-O2-C3
2	A	198	PEG	O2-C3-C4-O4

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	199	PEG	1	0
2	D	198	PEG	1	0
2	E	199	PEG	3	0
2	E	200	PEG	1	0
2	H	199	PEG	1	0
2	B	198	PEG	1	0
2	F	199	PEG	1	0
3	F	197	PGE	2	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	184/197 (93%)	0.29	0 100 100	15, 32, 48, 66	1 (0%)
1	B	184/197 (93%)	0.36	4 (2%) 62 66	12, 33, 52, 74	1 (0%)
1	C	183/197 (92%)	0.28	2 (1%) 78 80	19, 34, 50, 61	0
1	D	185/197 (93%)	0.29	2 (1%) 78 80	22, 34, 54, 68	0
1	E	184/197 (93%)	0.25	1 (0%) 87 89	22, 33, 53, 69	0
1	F	184/197 (93%)	0.25	0 100 100	24, 34, 51, 71	0
1	G	183/197 (92%)	0.32	2 (1%) 78 80	22, 35, 52, 61	0
1	H	184/197 (93%)	0.28	2 (1%) 78 80	23, 33, 53, 71	0
1	I	183/197 (92%)	0.28	2 (1%) 78 80	23, 35, 53, 67	0
1	J	182/197 (92%)	0.41	4 (2%) 62 66	26, 36, 53, 59	0
1	K	185/197 (93%)	0.32	4 (2%) 62 66	21, 36, 54, 69	0
1	L	183/197 (92%)	0.33	4 (2%) 62 66	26, 36, 53, 67	0
All	All	2204/2364 (93%)	0.31	27 (1%) 76 79	12, 34, 53, 74	2 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	21	ASP	2.9
1	J	34	ALA	2.8
1	J	30	VAL	2.6
1	D	16	LEU	2.6
1	J	192	VAL	2.6
1	L	5	ALA	2.5
1	K	193	PRO	2.5
1	I	17	ALA	2.4
1	G	28	LEU	2.4
1	B	194	LYS	2.4
1	D	4	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	28	LEU	2.3
1	L	16	LEU	2.3
1	I	193	PRO	2.3
1	K	21	ASP	2.3
1	G	17	ALA	2.2
1	L	17	ALA	2.2
1	H	194	LYS	2.2
1	C	192	VAL	2.1
1	B	193	PRO	2.1
1	E	30	VAL	2.1
1	K	30	VAL	2.1
1	B	18	ALA	2.1
1	B	16	LEU	2.0
1	H	193	PRO	2.0
1	J	13	VAL	2.0
1	C	17	ALA	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PEG	L	197	7/7	0.81	0.15	50,63,68,75	0
2	PEG	H	199	7/7	0.82	0.18	44,50,65,65	0
2	PEG	D	198	7/7	0.82	0.14	34,36,44,54	0
2	PEG	F	198	7/7	0.83	0.14	42,59,64,66	0
2	PEG	C	200	7/7	0.83	0.15	49,56,68,76	0
2	PEG	C	199	7/7	0.83	0.21	56,64,70,70	0
2	PEG	A	199	7/7	0.84	0.14	42,48,60,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PEG	G	198	7/7	0.84	0.13	44,48,61,63	0
2	PEG	B	198	7/7	0.84	0.13	42,44,53,58	0
2	PEG	B	199	7/7	0.84	0.15	41,47,63,63	0
2	PEG	F	199	7/7	0.85	0.16	48,51,64,68	0
2	PEG	E	198	7/7	0.85	0.13	46,46,51,52	0
2	PEG	A	198	7/7	0.86	0.13	36,47,56,56	0
2	PEG	K	197	7/7	0.86	0.12	46,51,54,56	0
2	PEG	K	198	7/7	0.86	0.13	49,54,63,64	0
2	PEG	G	199	7/7	0.86	0.18	64,67,68,70	0
2	PEG	J	198	7/7	0.88	0.12	38,41,47,53	0
2	PEG	J	199	7/7	0.88	0.14	51,53,58,62	0
2	PEG	E	199	7/7	0.88	0.13	43,46,52,54	0
2	PEG	C	198	7/7	0.88	0.11	27,34,44,47	0
2	PEG	I	197	7/7	0.88	0.12	45,50,55,56	0
2	PEG	A	197	7/7	0.89	0.11	35,40,43,51	0
3	PGE	B	197	10/10	0.89	0.13	34,46,52,56	0
3	PGE	C	197	10/10	0.89	0.12	38,45,50,50	0
3	PGE	E	197	10/10	0.89	0.12	36,40,45,46	0
2	PEG	H	198	7/7	0.90	0.08	38,42,47,49	0
3	PGE	F	197	10/10	0.90	0.12	30,39,53,55	0
3	PGE	G	197	10/10	0.90	0.14	47,59,65,66	0
3	PGE	H	197	10/10	0.90	0.11	39,42,46,55	0
2	PEG	E	200	7/7	0.91	0.12	46,49,55,57	0
3	PGE	D	197	10/10	0.91	0.11	31,38,48,49	0
2	PEG	J	197	7/7	0.91	0.10	37,42,45,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.