



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:57 AM UTC

PDB ID : 4XTS / pdb_00004xts
Title : Salmonella typhimurium AhpC T43A mutant
Authors : Perkins, A.; Nelson, K.; Parsonage, D.; Poole, L.; Karplus, P.A.
Deposited on : 2015-01-24
Resolution : 2.70 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

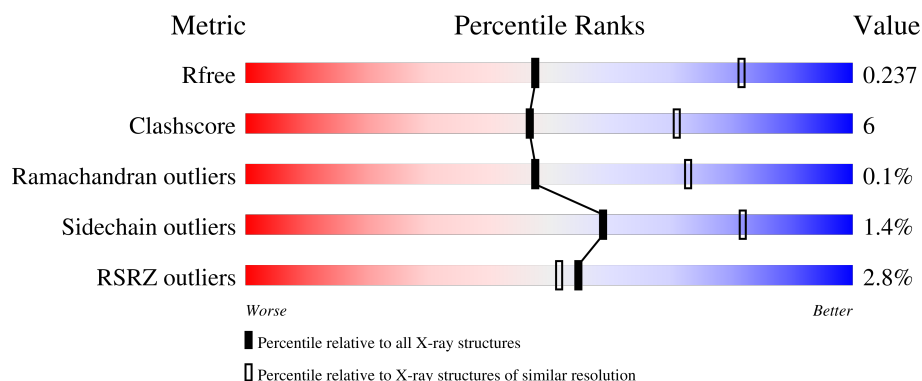
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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.



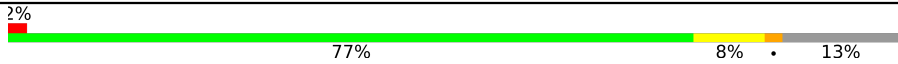
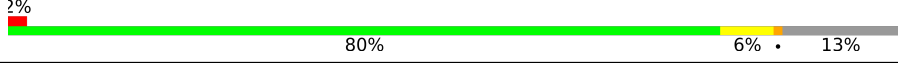
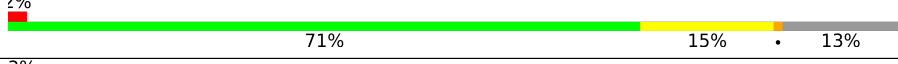
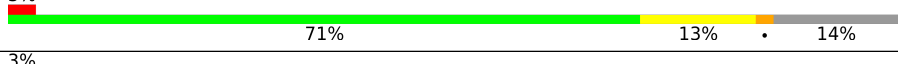
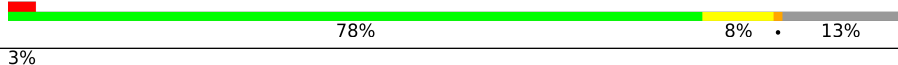
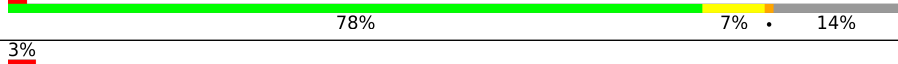
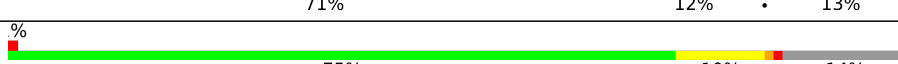
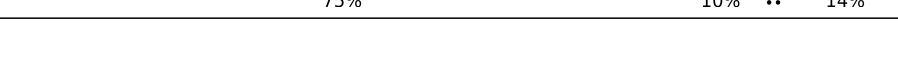
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	186	 2% 76% 9% • 14%
1	B	186	 3% 68% 19% 13%
1	C	186	 3% 70% 16% • 13%
1	D	186	 2% 72% 13% • 13%
1	E	186	 2% 75% 10% • 14%

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Mol	Chain	Length	Quality of chain
1	F	186	
1	G	186	
1	H	186	
1	I	186	
1	J	186	
1	K	186	
1	L	186	
1	M	186	
1	N	186	
1	O	186	
1	P	186	
1	Q	186	
1	R	186	
1	S	186	
1	T	186	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25877 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 Alkyl hydroperoxide reductase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	0	0	0
			1261	804	211	243	3			
1	B	162	Total	C	N	O	S	0	1	0
			1281	816	213	249	3			
1	C	162	Total	C	N	O	S	0	1	0
			1283	816	214	250	3			
1	D	161	Total	C	N	O	S	0	0	0
			1271	810	212	246	3			
1	E	160	Total	C	N	O	S	0	1	0
			1272	809	212	248	3			
1	F	161	Total	C	N	O	S	0	0	0
			1271	810	212	246	3			
1	G	161	Total	C	N	O	S	0	0	0
			1271	810	212	246	3			
1	H	161	Total	C	N	O	S	0	1	0
			1276	813	212	248	3			
1	I	161	Total	C	N	O	S	0	1	0
			1276	813	212	248	3			
1	J	161	Total	C	N	O	S	0	2	0
			1288	819	217	248	4			
1	K	160	Total	C	N	O	S	0	0	0
			1264	805	211	245	3			
1	L	162	Total	C	N	O	S	0	0	0
			1275	812	213	247	3			
1	M	161	Total	C	N	O	S	0	0	0
			1271	810	212	246	3			
1	N	160	Total	C	N	O	S	0	0	0
			1261	804	211	243	3			
1	O	160	Total	C	N	O	S	0	0	0
			1264	805	211	245	3			
1	P	160	Total	C	N	O	S	0	0	0
			1264	805	211	245	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	161	Total	C	N	O	S	0	0	0
			1271	810	212	246	3			
1	R	161	Total	C	N	O	S	0	0	0
			1271	810	212	246	3			
1	S	161	Total	C	N	O	S	0	0	0
			1271	810	212	246	3			
1	T	160	Total	C	N	O	S	0	0	0
			1264	805	211	245	3			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	ALA	THR	engineered mutation	UNP P0A251
B	43	ALA	THR	engineered mutation	UNP P0A251
C	43	ALA	THR	engineered mutation	UNP P0A251
D	43	ALA	THR	engineered mutation	UNP P0A251
E	43	ALA	THR	engineered mutation	UNP P0A251
F	43	ALA	THR	engineered mutation	UNP P0A251
G	43	ALA	THR	engineered mutation	UNP P0A251
H	43	ALA	THR	engineered mutation	UNP P0A251
I	43	ALA	THR	engineered mutation	UNP P0A251
J	43	ALA	THR	engineered mutation	UNP P0A251
K	43	ALA	THR	engineered mutation	UNP P0A251
L	43	ALA	THR	engineered mutation	UNP P0A251
M	43	ALA	THR	engineered mutation	UNP P0A251
N	43	ALA	THR	engineered mutation	UNP P0A251
O	43	ALA	THR	engineered mutation	UNP P0A251
P	43	ALA	THR	engineered mutation	UNP P0A251
Q	43	ALA	THR	engineered mutation	UNP P0A251
R	43	ALA	THR	engineered mutation	UNP P0A251
S	43	ALA	THR	engineered mutation	UNP P0A251
T	43	ALA	THR	engineered mutation	UNP P0A251

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total 2 Cl 2	0	0
2	B	1	Total 1 Cl 1	0	0
2	C	2	Total 2 Cl 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total 1	Cl 1	0	0
2	E	1	Total 1	Cl 1	0	0
2	F	1	Total 1	Cl 1	0	0
2	G	1	Total 1	Cl 1	0	0
2	H	2	Total 2	Cl 2	0	0
2	I	1	Total 1	Cl 1	0	0
2	J	2	Total 2	Cl 2	0	0
2	K	2	Total 2	Cl 2	0	0
2	L	2	Total 2	Cl 2	0	0
2	M	1	Total 1	Cl 1	0	0
2	N	1	Total 1	Cl 1	0	0
2	O	2	Total 2	Cl 2	0	0
2	P	1	Total 1	Cl 1	0	0
2	R	2	Total 2	Cl 2	0	0
2	S	1	Total 1	Cl 1	0	0
2	T	1	Total 1	Cl 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total 15	O 15	0	0
3	B	11	Total 11	O 11	0	0
3	C	27	Total 27	O 27	0	0

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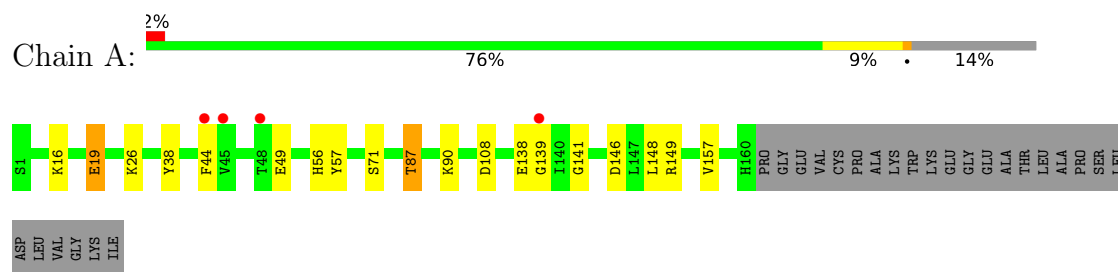
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	27	Total 27	O 27	0	0
3	E	32	Total 32	O 32	0	0
3	F	27	Total 28	O 28	0	1
3	G	21	Total 21	O 21	0	0
3	H	25	Total 25	O 25	0	0
3	I	12	Total 12	O 12	0	0
3	J	29	Total 29	O 29	0	0
3	K	15	Total 16	O 16	0	1
3	L	22	Total 23	O 23	0	1
3	M	9	Total 9	O 9	0	0
3	N	25	Total 26	O 26	0	1
3	O	16	Total 16	O 16	0	0
3	P	17	Total 17	O 17	0	0
3	Q	22	Total 22	O 22	0	0
3	R	15	Total 15	O 15	0	0
3	S	23	Total 23	O 23	0	0
3	T	30	Total 30	O 30	0	0

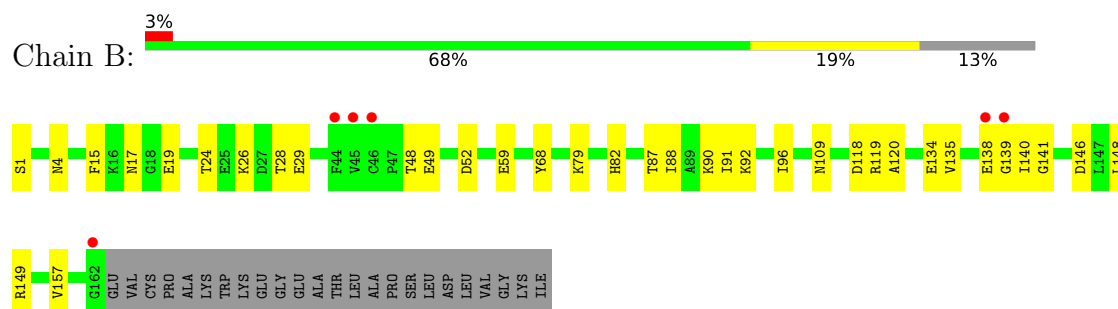
3 Residue-property plots [i](#)

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.

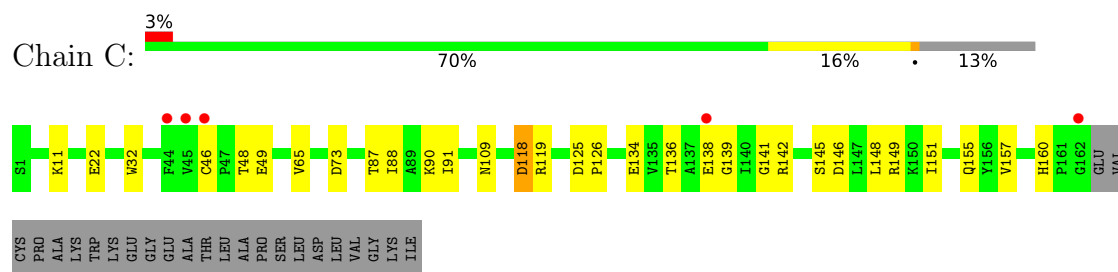
• Molecule 1: Alkyl hydroperoxide reductase subunit C



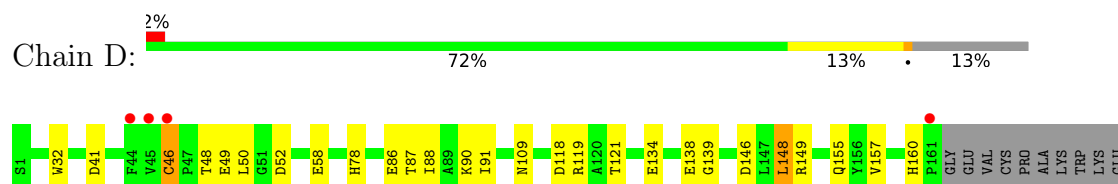
• Molecule 1: Alkyl hydroperoxide reductase subunit C



• Molecule 1: Alkyl hydroperoxide reductase subunit C



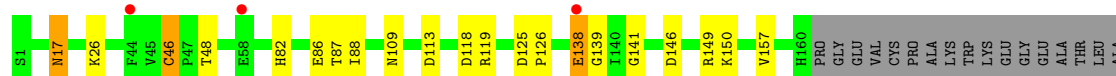
• Molecule 1: Alkyl hydroperoxide reductase subunit C



GLY
GLU
ALA
THR
LEU
ALA
PRO
SER
LEU
ASP
LEU
VAL
GLY
LYS
ILE

● Molecule 1: Alkyl hydroperoxide reductase subunit C

Chain E: 



PRO
SER
LEU
ASP
LEU
VAL
LYS
ILE

● Molecule 1: Alkyl hydroperoxide reductase subunit C

Chain F: 



LEU
VAL
GLY
LYS
ILE

● Molecule 1: Alkyl hydroperoxide reductase subunit C

Chain G: 



ALA
PRO
SER
LEU
LEU
VAL
GLY
LYS
ILE

● Molecule 1: Alkyl hydroperoxide reductase subunit C

Chain H: 



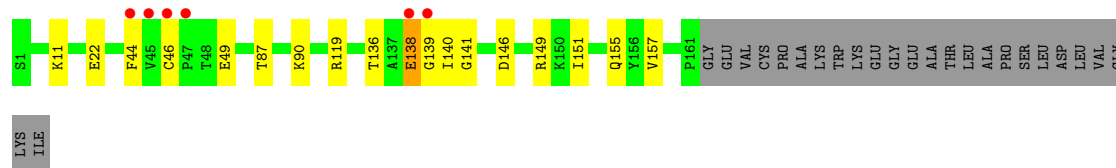
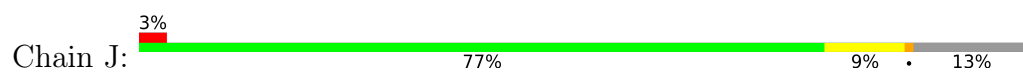
● Molecule 1: Alkyl hydroperoxide reductase subunit C

Chain I: 

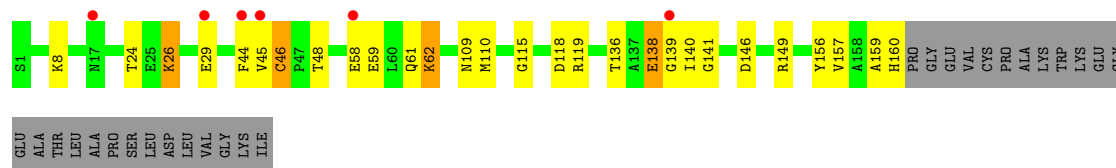


PRO
ALA
LYS
TRP
LYS
GLU
GLY
GLU
THR
LEU
ALA
PRO
SER
LEU
ASP
LEU
VAL
GLY
LYS
ILE

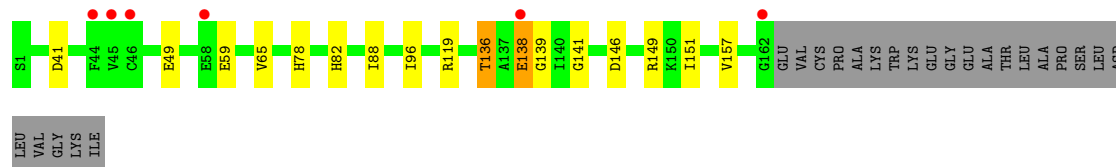
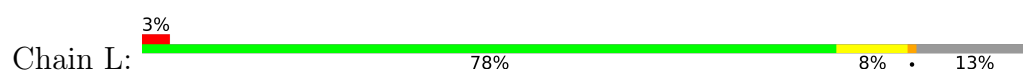
● Molecule 1: Alkyl hydroperoxide reductase subunit C



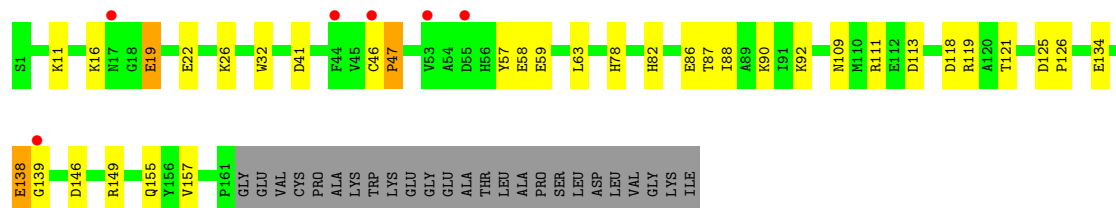
- Molecule 1: Alkyl hydroperoxide reductase subunit C



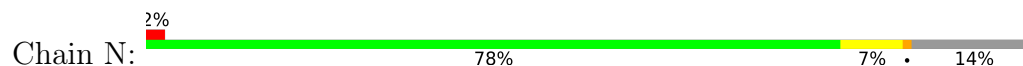
- Molecule 1: Alkyl hydroperoxide reductase subunit C



- Molecule 1: Alkyl hydroperoxide reductase subunit C

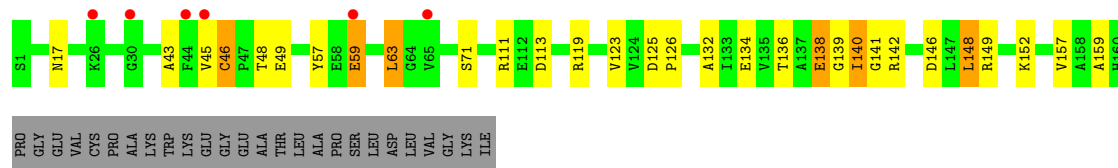


- Molecule 1: Alkyl hydroperoxide reductase subunit C

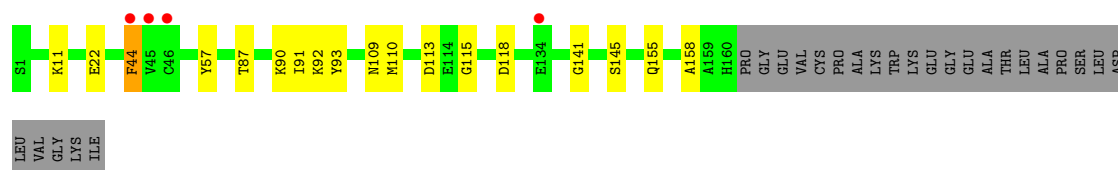
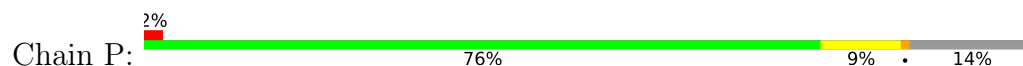


- Molecule 1: Alkyl hydroperoxide reductase subunit C

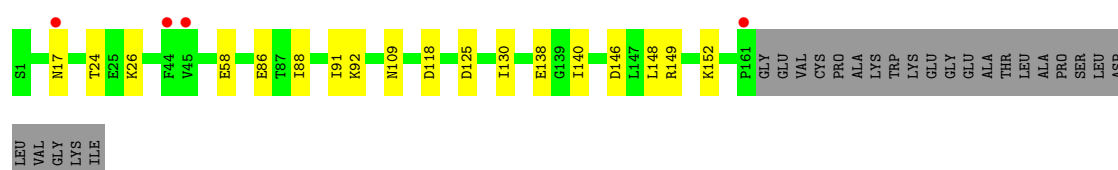
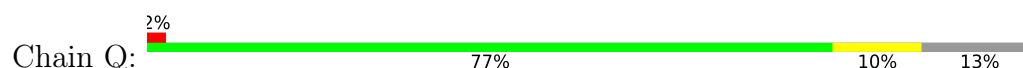




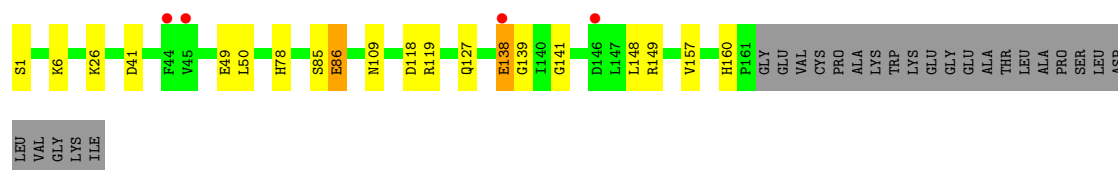
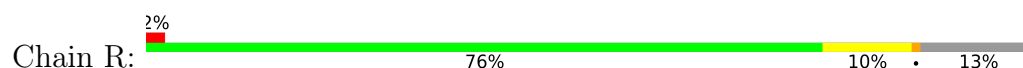
- Molecule 1: Alkyl hydroperoxide reductase subunit C



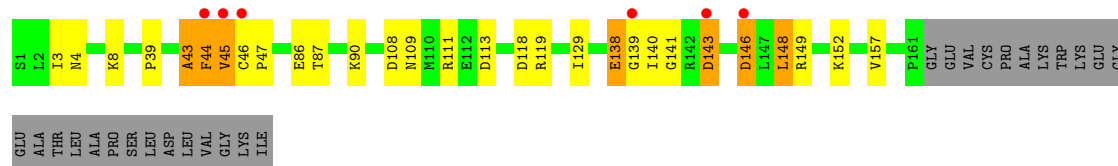
- Molecule 1: Alkyl hydroperoxide reductase subunit C



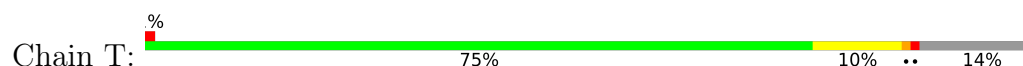
- Molecule 1: Alkyl hydroperoxide reductase subunit C



- Molecule 1: Alkyl hydroperoxide reductase subunit C



- Molecule 1: Alkyl hydroperoxide reductase subunit C





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	107.65Å 109.45Å 119.04Å 93.33° 110.02° 114.00°	Depositor
Resolution (Å)	63.51 – 2.70 63.51 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.8 (63.51-2.70) 95.8 (63.51-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.190 , 0.245 0.182 , 0.237	Depositor DCC
R_{free} test set	5943 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25877	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.72	0/1290	1.13	4/1747 (0.2%)
1	B	0.67	0/1314	1.14	3/1780 (0.2%)
1	C	0.70	0/1313	1.06	3/1779 (0.2%)
1	D	0.77	0/1301	1.21	4/1763 (0.2%)
1	E	0.79	0/1301	1.09	3/1762 (0.2%)
1	F	0.77	0/1301	1.21	9/1763 (0.5%)
1	G	0.77	0/1301	1.14	6/1763 (0.3%)
1	H	0.77	0/1309	1.09	3/1774 (0.2%)
1	I	0.76	0/1309	1.15	3/1774 (0.2%)
1	J	0.77	0/1318	1.07	2/1786 (0.1%)
1	K	0.71	0/1293	1.16	9/1751 (0.5%)
1	L	0.72	0/1305	1.07	3/1768 (0.2%)
1	M	0.71	0/1301	1.15	6/1763 (0.3%)
1	N	0.69	0/1290	1.11	3/1747 (0.2%)
1	O	0.72	0/1293	1.13	7/1751 (0.4%)
1	P	0.75	0/1293	1.08	1/1751 (0.1%)
1	Q	0.75	0/1301	1.12	3/1763 (0.2%)
1	R	0.70	0/1301	1.13	5/1763 (0.3%)
1	S	0.82	1/1301 (0.1%)	1.19	10/1763 (0.6%)
1	T	0.75	0/1293	1.17	8/1751 (0.5%)
All	All	0.74	1/26028 (0.0%)	1.13	95/35262 (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	M	0	1
1	S	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	45	VAL	CA-CB	5.37	1.61	1.54

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	138	GLU	N-CA-C	11.97	126.98	112.38
1	F	43	ALA	CA-C-N	-11.93	103.52	122.73
1	F	43	ALA	C-N-CA	-11.93	103.52	122.73
1	F	43	ALA	N-CA-C	-11.74	94.70	110.55
1	L	138	GLU	N-CA-C	11.06	126.14	112.87
1	D	46	CYS	CA-C-N	-10.42	106.81	119.84
1	D	46	CYS	C-N-CA	-10.42	106.81	119.84
1	I	138	GLU	N-CA-C	10.34	125.28	112.87
1	K	46	CYS	CA-C-N	-9.73	104.14	120.88
1	K	46	CYS	C-N-CA	-9.73	104.14	120.88
1	J	138	GLU	N-CA-C	9.49	123.90	111.75
1	A	138	GLU	N-CA-C	8.91	123.56	112.87
1	O	138	GLU	N-CA-C	8.85	123.49	112.87
1	Q	138	GLU	N-CA-C	8.68	123.28	112.87
1	D	160	HIS	N-CA-C	8.42	123.75	108.94
1	T	138	GLU	CA-C-N	8.33	135.37	120.79
1	T	138	GLU	C-N-CA	8.33	135.37	120.79
1	N	138	GLU	N-CA-C	8.26	122.78	112.87
1	C	138	GLU	N-CA-C	8.24	122.76	112.87
1	M	58	GLU	N-CA-C	-8.09	102.41	111.07
1	B	140	ILE	N-CA-C	7.86	118.82	106.88
1	B	138	GLU	N-CA-C	7.85	122.28	112.87
1	M	138	GLU	N-CA-C	7.69	122.10	112.87
1	H	44	PHE	CB-CA-C	-7.28	97.16	110.63
1	M	47	PRO	N-CA-C	7.22	122.22	112.48
1	A	57	TYR	N-CA-C	7.06	119.05	111.36
1	G	58	GLU	CB-CG-CD	7.06	124.60	112.60
1	G	138	GLU	N-CA-C	6.98	121.25	112.87
1	K	138	GLU	N-CA-C	6.95	121.21	112.87
1	G	58	GLU	CA-C-N	6.88	129.38	120.44
1	G	58	GLU	C-N-CA	6.88	129.38	120.44
1	R	138	GLU	N-CA-C	6.88	121.12	112.87
1	K	61	GLN	CA-CB-CG	-6.87	100.36	114.10
1	G	58	GLU	N-CA-C	6.79	118.34	111.07
1	T	58	GLU	CA-CB-CG	-6.77	100.56	114.10
1	M	57	TYR	N-CA-C	6.75	118.72	111.36
1	E	138	GLU	N-CA-C	6.75	125.18	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	138	GLU	N-CA-C	6.74	120.96	112.87
1	C	160	HIS	CA-C-N	6.64	127.00	119.83
1	C	160	HIS	C-N-CA	6.64	127.00	119.83
1	M	47	PRO	CB-CA-C	-6.63	104.20	112.89
1	H	138	GLU	N-CA-C	6.57	120.76	112.87
1	S	45	VAL	N-CA-C	6.55	122.95	109.34
1	T	139	GLY	N-CA-C	6.51	122.73	114.66
1	O	57	TYR	N-CA-C	6.50	118.45	111.36
1	A	49	GLU	N-CA-C	6.20	117.70	111.07
1	S	140	ILE	N-CA-C	6.16	116.98	107.99
1	O	140	ILE	N-CA-C	6.11	117.58	108.23
1	E	17	ASN	CB-CA-C	-6.08	98.31	110.42
1	F	43	ALA	CA-C-O	-6.03	114.70	121.81
1	S	138	GLU	N-CA-C	6.03	123.63	110.80
1	F	45	VAL	N-CA-C	-5.99	96.87	109.34
1	K	62	LYS	CA-CB-CG	5.93	125.96	114.10
1	G	46	CYS	N-CA-C	5.89	119.88	109.58
1	T	49	GLU	N-CA-C	5.82	117.29	111.07
1	R	85	SER	CA-C-N	5.80	128.06	120.28
1	R	85	SER	C-N-CA	5.80	128.06	120.28
1	R	160	HIS	N-CA-C	5.75	119.06	108.94
1	S	46	CYS	N-CA-C	-5.70	99.13	109.44
1	N	49	GLU	N-CA-C	5.67	117.14	111.07
1	Q	58	GLU	CA-CB-CG	5.64	125.39	114.10
1	S	45	VAL	CB-CA-C	-5.61	102.10	111.29
1	Q	140	ILE	N-CA-C	5.59	116.78	108.23
1	T	138	GLU	N-CA-C	5.56	122.65	110.80
1	R	148	LEU	N-CA-C	5.54	117.00	111.07
1	N	8	LYS	N-CA-CB	5.53	116.16	109.74
1	K	44	PHE	N-CA-C	-5.50	105.67	112.38
1	M	58	GLU	N-CA-CB	5.49	117.97	110.01
1	J	140	ILE	N-CA-C	5.46	115.97	107.99
1	S	45	VAL	CG1-CB-CG2	-5.45	98.81	110.80
1	F	49	GLU	N-CA-C	5.42	116.99	111.14
1	S	8	LYS	N-CA-CB	5.41	116.01	109.74
1	I	134	GLU	CB-CA-C	5.39	119.08	109.65
1	O	17	ASN	CB-CA-C	-5.37	104.26	111.89
1	H	86	GLU	CA-CB-CG	-5.37	103.36	114.10
1	K	62	LYS	N-CA-C	-5.35	106.01	112.54
1	L	59	GLU	N-CA-C	5.27	116.71	111.07
1	S	143	ASP	CB-CA-C	5.24	118.69	110.19
1	T	8	LYS	CA-C-N	5.21	125.13	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	8	LYS	C-N-CA	5.21	125.13	119.76
1	O	46	CYS	CA-C-N	-5.13	112.06	120.88
1	O	46	CYS	C-N-CA	-5.13	112.06	120.88
1	E	46	CYS	N-CA-C	5.13	116.86	109.48
1	S	43	ALA	N-CA-C	5.12	117.47	110.55
1	B	19	GLU	N-CA-C	5.09	117.41	109.52
1	K	8	LYS	CA-C-N	5.08	125.00	119.76
1	K	8	LYS	C-N-CA	5.08	125.00	119.76
1	I	160	HIS	N-CA-C	5.07	117.86	108.94
1	A	87	THR	CB-CA-C	-5.06	102.91	110.90
1	L	136	THR	N-CA-C	5.04	116.85	109.24
1	O	17	ASN	N-CA-C	5.03	118.34	111.39
1	S	146	ASP	CB-CA-C	-5.02	102.31	110.85
1	F	8	LYS	CA-C-N	5.01	124.92	119.76
1	F	8	LYS	C-N-CA	5.01	124.92	119.76
1	P	44	PHE	N-CA-C	-5.01	106.43	112.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	19	GLU	Sidechain
1	S	43	ALA	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	1261	0	1219	13	0
1	B	1281	0	1237	23	0
1	C	1283	0	1234	18	0
1	D	1271	0	1228	18	0
1	E	1272	0	1224	18	0
1	F	1271	0	1228	12	0
1	G	1271	0	1228	24	0
1	H	1276	0	1232	11	0
1	I	1276	0	1232	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	1288	0	1245	18	0
1	K	1264	0	1221	20	0
1	L	1275	0	1231	12	0
1	M	1271	0	1228	23	0
1	N	1261	0	1219	9	0
1	O	1264	0	1221	20	0
1	P	1264	0	1221	11	0
1	Q	1271	0	1228	9	0
1	R	1271	0	1228	14	0
1	S	1271	0	1228	26	0
1	T	1264	0	1221	16	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	2	0	0	0	0
2	I	1	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	2	0	0	0	0
2	P	1	0	0	0	0
2	R	2	0	0	1	0
2	S	1	0	0	0	0
2	T	1	0	0	0	0
3	A	15	0	0	0	0
3	B	11	0	0	1	0
3	C	27	0	0	1	0
3	D	27	0	0	0	0
3	E	32	0	0	0	0
3	F	28	0	0	0	0
3	G	21	0	0	0	0
3	H	25	0	0	0	0
3	I	12	0	0	0	0
3	J	29	0	0	0	0
3	K	16	0	0	0	0
3	L	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	M	9	0	0	0	0
3	N	26	0	0	0	0
3	O	16	0	0	0	0
3	P	17	0	0	1	0
3	Q	22	0	0	1	0
3	R	15	0	0	0	0
3	S	23	0	0	1	0
3	T	30	0	0	2	0
All	All	25877	0	24553	284	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 6.

All (284) 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:H:157:VAL:HG11	1:I:139:GLY:HA3	1.43	1.00
1:S:4:ASN:ND2	3:S:311:HOH:O	1.98	0.96
1:A:157:VAL:HG11	1:B:139:GLY:HA3	1.48	0.95
1:F:157:VAL:HG11	1:G:139:GLY:HA3	1.46	0.93
1:C:146:ASP:OD1	1:C:149:ARG:NH1	2.03	0.92
1:A:139:GLY:HA3	1:B:157:VAL:HG11	1.53	0.91
1:E:139:GLY:HA3	1:J:157:VAL:HG11	1.54	0.88
1:R:141:GLY:O	1:S:149:ARG:NH2	2.07	0.87
1:S:44:PHE:HD2	1:S:45:VAL:HG23	1.41	0.85
1:K:157:VAL:HG11	1:L:139:GLY:HA3	1.58	0.85
1:O:139:GLY:HA3	1:T:157:VAL:HG11	1.60	0.84
1:E:157:VAL:HG21	1:J:139:GLY:HA3	1.60	0.83
1:B:146:ASP:OD1	1:B:149:ARG:NH1	2.10	0.83
1:G:59:GLU:O	1:G:62:LYS:HG2	1.79	0.82
1:S:143:ASP:OD1	1:S:146:ASP:HB2	1.79	0.81
1:K:139:GLY:HA3	1:L:157:VAL:HG21	1.61	0.80
1:A:146:ASP:OD1	1:A:149:ARG:NH1	2.15	0.79
1:M:157:VAL:HG11	1:N:139:GLY:HA3	1.65	0.79
1:N:138:GLU:H	1:N:138:GLU:CD	1.91	0.78
1:F:149:ARG:NH2	1:G:141:GLY:O	2.17	0.77
1:D:146:ASP:OD1	1:D:149:ARG:NH1	2.18	0.76
1:E:141:GLY:O	1:J:149:ARG:NH2	2.18	0.76
1:I:16:LYS:HE2	1:I:21:ILE:HD13	1.67	0.76
1:H:149:ARG:NH2	1:I:141:GLY:O	2.18	0.75
1:C:141:GLY:O	1:D:149:ARG:NH2	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:58:GLU:CG	1:G:59:GLU:H	2.01	0.74
1:K:149:ARG:NH2	1:L:141:GLY:O	2.19	0.74
1:C:157:VAL:HG11	1:D:139:GLY:HA3	1.69	0.74
1:T:146:ASP:OD1	1:T:149:ARG:NH1	2.20	0.73
1:L:146:ASP:OD1	1:L:149:ARG:NH1	2.21	0.73
1:M:139:GLY:HA3	1:N:157:VAL:HG11	1.71	0.73
1:O:146:ASP:OD1	1:O:149:ARG:NH1	2.21	0.73
1:M:149:ARG:NH2	1:N:141:GLY:O	2.23	0.72
1:O:49:GLU:OE2	1:O:119:ARG:NH2	2.23	0.72
1:M:111:ARG:NH1	1:M:138:GLU:OE2	2.22	0.72
1:Q:146:ASP:OD1	1:Q:149:ARG:NH1	2.22	0.71
1:F:139:GLY:HA3	1:G:157:VAL:HG11	1.71	0.71
1:R:149:ARG:NH2	1:S:141:GLY:O	2.24	0.71
1:J:146:ASP:OD1	1:J:149:ARG:NH1	2.26	0.69
1:A:149:ARG:NH2	1:B:141:GLY:O	2.26	0.69
1:R:86:GLU:CD	1:R:86:GLU:H	1.96	0.69
1:T:143:ASP:OD1	3:T:301:HOH:O	2.10	0.69
1:G:58:GLU:HG3	1:G:59:GLU:N	2.09	0.68
1:S:44:PHE:CD2	1:S:45:VAL:HG23	2.26	0.67
1:O:157:VAL:HG21	1:T:139:GLY:HA3	1.75	0.67
1:I:146[B]:ASP:OD1	1:I:149:ARG:NH1	2.29	0.66
1:F:110:MET:HE1	1:F:115:GLY:HA2	1.78	0.66
1:E:146[B]:ASP:OD2	1:E:149:ARG:NH1	2.28	0.66
1:J:119[A]:ARG:NH1	1:J:136:THR:OG1	2.29	0.66
1:K:58:GLU:OE1	1:K:58:GLU:N	2.30	0.64
1:L:49:GLU:OE2	1:L:119:ARG:NH2	2.30	0.64
1:C:139:GLY:HA3	1:D:157:VAL:HG21	1.78	0.64
1:F:25:GLU:OE2	1:F:26:LYS:HE3	1.98	0.64
1:O:43:ALA:HB3	1:O:45:VAL:HG22	1.80	0.64
1:G:44:PHE:CZ	1:H:20:PHE:HE2	2.17	0.63
1:J:119[B]:ARG:NH1	1:J:138:GLU:OE2	2.31	0.63
1:H:141:GLY:O	1:I:149:ARG:NH2	2.32	0.63
1:E:157:VAL:HG21	1:J:139:GLY:CA	2.29	0.63
1:A:87:THR:O	1:A:90:LYS:HG2	1.99	0.63
1:G:58:GLU:CG	1:G:59:GLU:N	2.59	0.63
1:B:88:ILE:HG23	1:B:91:ILE:HD12	1.81	0.62
1:O:134:GLU:OE2	1:O:142:ARG:HG2	1.99	0.62
1:I:62:LYS:HD2	1:I:62:LYS:N	2.13	0.62
1:S:148:LEU:HD21	1:S:152:LYS:HE3	1.80	0.62
1:G:159:ALA:HB1	1:O:159:ALA:HA	1.82	0.62
1:O:59:GLU:O	1:O:63:LEU:HD13	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:49:GLU:OE2	1:J:119[A]:ARG:NH2	2.33	0.61
1:K:146:ASP:OD1	1:K:149:ARG:NH1	2.34	0.61
1:R:139:GLY:HA3	1:S:157:VAL:HG11	1.83	0.61
1:G:44:PHE:HZ	1:H:20:PHE:HE2	1.49	0.60
1:K:58:GLU:HG2	1:K:59:GLU:N	2.16	0.60
1:Q:148:LEU:HG	1:Q:152:LYS:HE3	1.83	0.60
1:R:157:VAL:HG11	1:S:139:GLY:HA3	1.83	0.59
1:B:68:TYR:HB3	1:B:96:ILE:HD12	1.83	0.59
1:D:46:CYS:O	1:D:48:THR:N	2.36	0.59
1:G:58:GLU:HG3	1:G:59:GLU:H	1.62	0.58
1:D:87:THR:O	1:D:90:LYS:HG2	2.03	0.58
1:R:138:GLU:CD	1:R:138:GLU:H	2.12	0.58
1:F:157:VAL:HG11	1:G:139:GLY:CA	2.26	0.58
1:Q:109:ASN:OD1	1:Q:118:ASP:HB2	2.03	0.58
1:D:121:THR:HB	1:D:134:GLU:HG2	1.84	0.58
1:H:139:GLY:HA3	1:I:157:VAL:HG21	1.86	0.57
1:O:141:GLY:O	1:T:149:ARG:NH2	2.37	0.57
1:B:26:LYS:O	1:B:29:GLU:HG2	2.03	0.57
1:G:138:GLU:HG3	1:G:138:GLU:O	2.04	0.57
1:B:49:GLU:OE2	1:B:119:ARG:NH1	2.38	0.57
1:G:146:ASP:OD1	1:G:149:ARG:NH1	2.38	0.57
1:M:16:LYS:O	1:M:19:GLU:HG2	2.05	0.56
1:E:125:ASP:HB2	1:E:126:PRO:CD	2.36	0.56
1:K:141:GLY:O	1:L:149:ARG:NH2	2.39	0.56
1:A:141:GLY:O	1:B:149:ARG:NH2	2.37	0.56
1:K:46:CYS:O	1:K:48:THR:N	2.36	0.56
1:S:87:THR:O	1:S:90:LYS:HG2	2.06	0.55
1:M:32:TRP:CD1	1:M:155:GLN:HE21	2.24	0.55
1:S:143:ASP:OD1	1:S:146:ASP:CB	2.51	0.55
1:I:111:ARG:NH1	1:I:138:GLU:OE2	2.40	0.55
1:P:109:ASN:OD1	1:P:118:ASP:HB2	2.07	0.54
1:G:58:GLU:HG2	1:G:59:GLU:H	1.70	0.54
1:E:86:GLU:CD	1:E:86:GLU:H	2.05	0.54
1:O:149:ARG:NH2	1:T:141:GLY:O	2.41	0.54
1:F:87:THR:O	1:F:90:LYS:HG2	2.08	0.54
1:S:44:PHE:CD2	1:S:45:VAL:N	2.76	0.54
1:L:119:ARG:NH1	1:L:136:THR:OG1	2.41	0.54
1:N:109:ASN:OD1	1:N:118:ASP:HB2	2.08	0.54
3:Q:215:HOH:O	2:R:202:CL:CL	2.55	0.53
1:C:119:ARG:NH1	1:C:136:THR:OG1	2.41	0.53
1:P:44:PHE:HD2	1:P:44:PHE:O	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:119:ARG:HD2	1:K:138:GLU:OE2	2.08	0.53
1:K:156:TYR:CZ	1:K:160:HIS:HD2	2.26	0.53
1:S:111:ARG:NE	1:S:118:ASP:OD1	2.27	0.53
1:A:56:HIS:ND1	1:A:148:LEU:HD12	2.25	0.52
1:T:156:TYR:CZ	1:T:160:HIS:HD2	2.28	0.52
1:M:86:GLU:OE1	1:M:86:GLU:N	2.38	0.52
1:G:44:PHE:HZ	1:H:20:PHE:CE2	2.28	0.52
1:D:32:TRP:CD1	1:D:155:GLN:HE21	2.27	0.52
1:H:109:ASN:OD1	1:H:118:ASP:HB2	2.09	0.52
1:B:87:THR:O	1:B:90:LYS:HG2	2.09	0.52
1:Q:86:GLU:OE1	1:Q:86:GLU:HA	2.08	0.52
1:B:28:THR:HA	3:B:310:HOH:O	2.10	0.52
1:L:41:ASP:OD2	1:L:78:HIS:HD2	1.92	0.52
1:A:44:PHE:HE2	1:F:20:PHE:HE2	1.58	0.52
1:A:16:LYS:O	1:A:19:GLU:HG3	2.10	0.51
1:H:87:THR:O	1:H:90:LYS:HG2	2.10	0.51
1:R:1:SER:N	1:S:108:ASP:O	2.42	0.51
1:F:43:ALA:HB3	1:F:45:VAL:HG22	1.92	0.51
1:K:109:ASN:OD1	1:K:118:ASP:HB2	2.11	0.51
1:M:11:LYS:HE3	1:M:22:GLU:CD	2.36	0.51
1:M:86:GLU:HG2	1:M:87:THR:N	2.25	0.51
1:I:43:ALA:HB3	1:I:45:VAL:HG22	1.93	0.51
1:I:87:THR:O	1:I:90:LYS:HG2	2.10	0.51
1:D:109:ASN:OD1	1:D:118:ASP:HB2	2.11	0.51
1:M:146:ASP:OD1	1:M:149:ARG:NH1	2.44	0.51
1:I:11:LYS:HG3	1:I:24:THR:HG22	1.93	0.50
1:I:20:PHE:HE2	1:J:44:PHE:CZ	2.29	0.50
1:S:148:LEU:CD2	1:S:152:LYS:HE3	2.42	0.50
1:I:49:GLU:OE1	1:I:119:ARG:NH2	2.45	0.50
1:G:87:THR:O	1:G:90:LYS:HG2	2.11	0.50
1:M:59:GLU:O	1:M:63:LEU:HD12	2.11	0.50
1:D:49:GLU:OE1	1:D:119:ARG:NH2	2.45	0.49
1:M:139:GLY:CA	1:N:157:VAL:HG11	2.41	0.49
1:M:121:THR:HB	1:M:134:GLU:HG2	1.92	0.49
1:F:141:GLY:O	1:G:149:ARG:NH2	2.42	0.49
1:R:6:LYS:HE3	1:R:127:GLN:O	2.11	0.49
1:Q:24:THR:OG1	1:Q:26:LYS:HB2	2.13	0.49
1:O:111:ARG:NH1	1:O:138:GLU:OE2	2.34	0.49
1:P:158:ALA:O	3:P:308:HOH:O	2.20	0.49
1:D:49:GLU:HA	1:D:52:ASP:OD1	2.12	0.48
1:K:139:GLY:CA	1:L:157:VAL:HG21	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:87:THR:O	1:P:90:LYS:HG2	2.13	0.48
1:T:156:TYR:CZ	1:T:160:HIS:CD2	3.02	0.48
1:G:51:GLY:O	1:G:54:ALA:HB3	2.13	0.48
1:P:11:LYS:HE2	1:P:22:GLU:OE1	2.14	0.48
1:C:151:ILE:O	1:C:155:GLN:HG3	2.12	0.48
1:J:11:LYS:HE2	1:J:22:GLU:CD	2.39	0.47
1:P:91:ILE:C	1:P:92:LYS:HD3	2.39	0.47
1:T:159:ALA:C	1:T:160:HIS:HD1	2.23	0.47
1:I:49:GLU:CD	1:I:119:ARG:HH22	2.22	0.47
1:K:159:ALA:C	1:K:160:HIS:HD1	2.21	0.47
1:C:46:CYS:C	1:C:48:THR:H	2.23	0.47
1:I:109:ASN:OD1	1:I:118:ASP:HB2	2.14	0.47
1:P:57:TYR:CE1	1:P:93:TYR:HB3	2.49	0.47
1:I:32:TRP:CE2	1:I:126:PRO:HD3	2.50	0.47
1:S:109:ASN:OD1	1:S:118:ASP:HB2	2.15	0.47
1:C:11:LYS:HE3	1:C:22:GLU:OE2	2.15	0.47
1:D:148:LEU:HA	1:D:148:LEU:HD23	1.57	0.47
1:T:127:GLN:HB3	3:T:312:HOH:O	2.14	0.47
1:D:49:GLU:CD	1:D:119:ARG:NH2	2.72	0.47
1:J:151:ILE:O	1:J:155:GLN:HG3	2.15	0.47
1:O:49:GLU:CD	1:O:119:ARG:HH22	2.23	0.46
1:F:49:GLU:CD	1:F:119:ARG:NH1	2.73	0.46
1:G:76:PHE:HE1	1:H:44:PHE:CE1	2.32	0.46
1:T:87:THR:O	1:T:90:LYS:HG2	2.15	0.46
1:B:109:ASN:OD1	1:B:118:ASP:HB2	2.15	0.46
1:S:39:PRO:HD3	1:S:119:ARG:HG2	1.97	0.46
1:E:113:ASP:OD1	1:E:113:ASP:N	2.46	0.46
1:O:46:CYS:O	1:O:48:THR:N	2.40	0.46
1:R:157:VAL:HG11	1:S:139:GLY:CA	2.45	0.46
1:C:73:ASP:OD1	3:C:326:HOH:O	2.20	0.46
1:J:87:THR:O	1:J:90:LYS:HG2	2.16	0.46
1:K:58:GLU:CG	1:K:59:GLU:N	2.77	0.46
1:P:141:GLY:O	1:Q:149:ARG:NH2	2.44	0.46
1:B:15:PHE:CE1	1:B:79:LYS:HG3	2.51	0.46
1:O:157:VAL:CG2	1:T:139:GLY:HA3	2.46	0.46
1:Q:88:ILE:HG23	1:Q:91:ILE:HD12	1.99	0.45
1:S:45:VAL:CG1	1:S:47:PRO:HA	2.45	0.45
1:J:11:LYS:HE2	1:J:22:GLU:OE2	2.16	0.45
1:M:41:ASP:OD2	1:M:78:HIS:ND1	2.33	0.45
1:I:49:GLU:CD	1:I:119:ARG:NH2	2.75	0.45
1:R:109:ASN:OD1	1:R:118:ASP:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:LYS:HB2	1:E:26:LYS:HE2	1.71	0.45
1:E:46:CYS:O	1:E:48:THR:N	2.45	0.45
1:M:82:HIS:HA	1:M:88:ILE:HG22	1.98	0.45
1:S:143:ASP:OD1	1:S:143:ASP:O	2.34	0.45
1:M:87:THR:O	1:M:90:LYS:HG2	2.17	0.44
1:C:125:ASP:HB2	1:C:126:PRO:CD	2.47	0.44
1:E:86:GLU:HG2	1:E:87:THR:H	1.82	0.44
1:K:110:MET:HE3	1:K:115:GLY:HA2	2.00	0.44
1:G:144:ALA:O	1:G:147:LEU:HB3	2.17	0.44
1:T:156:TYR:CE2	1:T:160:HIS:HD2	2.36	0.44
1:E:82:HIS:HA	1:E:88:ILE:HG22	1.99	0.44
1:M:157:VAL:HG11	1:N:139:GLY:CA	2.43	0.44
1:A:108:ASP:O	1:B:1:SER:N	2.51	0.44
1:N:87:THR:O	1:N:90:LYS:HG2	2.18	0.44
1:B:48:THR:O	1:B:52:ASP:HB2	2.18	0.44
1:R:49:GLU:CD	1:R:119:ARG:HH22	2.26	0.44
1:P:155:GLN:O	1:P:158:ALA:HB3	2.18	0.44
1:D:50:LEU:HD23	1:D:50:LEU:HA	1.86	0.44
1:M:113:ASP:OD1	1:M:113:ASP:N	2.48	0.44
1:B:148:LEU:HD23	1:B:148:LEU:HA	1.87	0.43
1:E:157:VAL:HG11	1:J:139:GLY:HA3	2.00	0.43
1:I:20:PHE:CE2	1:J:44:PHE:HZ	2.37	0.43
1:R:50:LEU:HD23	1:R:50:LEU:HA	1.88	0.43
1:I:58:GLU:O	1:I:62:LYS:HD3	2.17	0.43
1:B:49:GLU:CD	1:B:119:ARG:HH12	2.26	0.43
1:O:148:LEU:HD22	1:O:152:LYS:HE3	2.01	0.43
1:I:11:LYS:HE3	1:I:22:GLU:OE2	2.19	0.43
1:B:17:ASN:ND2	1:B:92:LYS:O	2.52	0.43
1:C:148:LEU:HD12	1:C:148:LEU:HA	1.78	0.43
1:K:24:THR:OG1	1:K:26:LYS:HG3	2.18	0.43
1:S:113:ASP:OD1	1:S:113:ASP:N	2.50	0.43
1:M:119:ARG:HD2	1:M:138:GLU:OE2	2.18	0.43
1:S:3:ILE:HD12	1:S:3:ILE:HA	1.91	0.43
1:D:41:ASP:OD2	1:D:78:HIS:ND1	2.41	0.43
1:O:125:ASP:HB2	1:O:126:PRO:CD	2.49	0.43
1:L:82:HIS:HA	1:L:88:ILE:HG22	2.01	0.42
1:O:123:VAL:HB	1:O:132:ALA:HB3	2.00	0.42
1:Q:125:ASP:OD1	1:Q:125:ASP:C	2.62	0.42
1:A:139:GLY:CA	1:B:157:VAL:HG11	2.35	0.42
1:C:87:THR:O	1:C:90:LYS:HG2	2.18	0.42
1:O:113:ASP:OD1	1:O:113:ASP:N	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:49:GLU:OE2	1:F:119:ARG:NH1	2.53	0.42
1:R:41:ASP:OD2	1:R:78:HIS:ND1	2.39	0.42
1:B:120:ALA:HB2	1:B:135:VAL:HG13	2.01	0.42
1:C:88:ILE:HG23	1:C:91:ILE:HD12	2.00	0.42
1:K:159:ALA:C	1:K:160:HIS:ND1	2.77	0.42
1:E:86:GLU:HG2	1:E:87:THR:N	2.34	0.42
1:C:109:ASN:OD1	1:C:118[B]:ASP:HB2	2.20	0.42
1:S:143:ASP:OD1	1:S:143:ASP:C	2.63	0.42
1:T:56:HIS:CD2	1:T:148:LEU:HD12	2.54	0.42
1:T:159:ALA:C	1:T:160:HIS:ND1	2.78	0.42
1:C:134:GLU:OE2	1:C:142:ARG:HG2	2.20	0.41
1:O:49:GLU:CD	1:O:119:ARG:NH2	2.78	0.41
1:E:125:ASP:HB2	1:E:126:PRO:HD2	2.03	0.41
1:M:125:ASP:OD1	1:M:125:ASP:C	2.64	0.41
1:E:109:ASN:OD1	1:E:118:ASP:HB2	2.19	0.41
1:P:110:MET:HE3	1:P:115:GLY:HA2	2.03	0.41
1:D:50:LEU:HB3	1:D:91:ILE:HD11	2.02	0.41
1:J:119[A]:ARG:HD2	1:J:138:GLU:OE2	2.20	0.41
1:C:32:TRP:CE2	1:C:126:PRO:HD3	2.55	0.41
1:C:49:GLU:CD	1:C:119:ARG:NH2	2.78	0.41
1:O:136:THR:HB	1:O:140:ILE:HB	2.01	0.41
1:I:11:LYS:HE3	1:I:22:GLU:CD	2.46	0.41
1:J:49:GLU:CD	1:J:119[A]:ARG:NH2	2.79	0.41
1:M:109:ASN:OD1	1:M:118:ASP:HB2	2.20	0.41
1:E:119:ARG:HD2	1:E:138:GLU:OE2	2.20	0.41
1:I:32:TRP:CE3	1:I:125:ASP:HA	2.56	0.41
1:P:113:ASP:OD1	1:P:113:ASP:N	2.51	0.41
1:Q:17:ASN:OD1	1:Q:92:LYS:HD3	2.21	0.41
1:A:38:TYR:CZ	1:A:71:SER:HB3	2.56	0.41
1:G:32:TRP:HB2	1:G:65:VAL:HG22	2.02	0.41
1:K:58:GLU:CG	1:K:59:GLU:H	2.34	0.41
1:M:46:CYS:HA	1:M:47:PRO:HD3	2.00	0.41
1:S:129:ILE:HD13	1:S:129:ILE:HA	1.88	0.41
1:D:49:GLU:CD	1:D:119:ARG:HH22	2.29	0.41
1:K:136:THR:HB	1:K:140:ILE:HB	2.03	0.41
1:L:65:VAL:HG21	1:L:151:ILE:HG21	2.03	0.41
1:R:139:GLY:CA	1:S:157:VAL:HG11	2.50	0.41
1:E:149:ARG:NH2	1:J:141:GLY:O	2.54	0.40
1:G:86:GLU:OE1	1:G:86:GLU:HA	2.20	0.40
1:L:78:HIS:HE1	1:L:96:ILE:O	2.04	0.40
1:T:137:ALA:HB3	1:T:140:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:ILE:HG23	1:D:91:ILE:HD12	2.04	0.40
1:K:58:GLU:HG2	1:K:59:GLU:H	1.86	0.40
1:A:149:ARG:HH11	1:A:149:ARG:HD3	1.76	0.40
1:B:24:THR:OG1	1:B:26:LYS:HB2	2.20	0.40
1:B:120:ALA:HA	1:B:134:GLU:O	2.21	0.40
1:C:65:VAL:HG21	1:C:151:ILE:HG21	2.02	0.40
1:I:113:ASP:OD1	1:I:113:ASP:N	2.50	0.40
1:M:125:ASP:HB2	1:M:126:PRO:CD	2.51	0.40
1:N:50:LEU:HB3	1:N:91:ILE:HD11	2.04	0.40
1:B:82:HIS:HA	1:B:88:ILE:HG22	2.02	0.40
1:G:136:THR:HB	1:G:140:ILE:HB	2.03	0.40
1:H:146[B]:ASP:OD2	1:H:149:ARG:NH1	2.55	0.40
1:S:86:GLU:OE2	1:S:86:GLU:HA	2.21	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	158/186 (85%)	155 (98%)	3 (2%)	0	100	100
1	B	161/186 (87%)	160 (99%)	1 (1%)	0	100	100
1	C	161/186 (87%)	158 (98%)	3 (2%)	0	100	100
1	D	159/186 (86%)	157 (99%)	2 (1%)	0	100	100
1	E	159/186 (86%)	156 (98%)	2 (1%)	1 (1%)	21	44
1	F	159/186 (86%)	156 (98%)	3 (2%)	0	100	100
1	G	159/186 (86%)	156 (98%)	3 (2%)	0	100	100
1	H	160/186 (86%)	157 (98%)	3 (2%)	0	100	100
1	I	160/186 (86%)	157 (98%)	3 (2%)	0	100	100
1	J	161/186 (87%)	159 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	158/186 (85%)	155 (98%)	3 (2%)	0	100	100
1	L	160/186 (86%)	157 (98%)	3 (2%)	0	100	100
1	M	159/186 (86%)	156 (98%)	3 (2%)	0	100	100
1	N	158/186 (85%)	155 (98%)	3 (2%)	0	100	100
1	O	158/186 (85%)	155 (98%)	3 (2%)	0	100	100
1	P	158/186 (85%)	156 (99%)	2 (1%)	0	100	100
1	Q	159/186 (86%)	156 (98%)	3 (2%)	0	100	100
1	R	159/186 (86%)	156 (98%)	3 (2%)	0	100	100
1	S	159/186 (86%)	155 (98%)	3 (2%)	1 (1%)	21	44
1	T	158/186 (85%)	155 (98%)	2 (1%)	1 (1%)	21	44
All	All	3183/3720 (86%)	3127 (98%)	53 (2%)	3 (0%)	48	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	T	138	GLU
1	E	17	ASN
1	S	44	PHE

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	132/153 (86%)	130 (98%)	2 (2%)	57	81
1	B	135/153 (88%)	132 (98%)	3 (2%)	45	74
1	C	135/153 (88%)	132 (98%)	3 (2%)	45	74
1	D	134/153 (88%)	131 (98%)	3 (2%)	45	74
1	E	134/153 (88%)	133 (99%)	1 (1%)	76	90
1	F	134/153 (88%)	132 (98%)	2 (2%)	57	81
1	G	134/153 (88%)	133 (99%)	1 (1%)	76	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	135/153 (88%)	134 (99%)	1 (1%)	76	90
1	I	135/153 (88%)	134 (99%)	1 (1%)	76	90
1	J	136/153 (89%)	134 (98%)	2 (2%)	57	81
1	K	133/153 (87%)	129 (97%)	4 (3%)	36	66
1	L	134/153 (88%)	133 (99%)	1 (1%)	76	90
1	M	134/153 (88%)	132 (98%)	2 (2%)	57	81
1	N	132/153 (86%)	130 (98%)	2 (2%)	57	81
1	O	133/153 (87%)	129 (97%)	4 (3%)	36	66
1	P	133/153 (87%)	132 (99%)	1 (1%)	73	88
1	Q	134/153 (88%)	133 (99%)	1 (1%)	76	90
1	R	134/153 (88%)	132 (98%)	2 (2%)	57	81
1	S	134/153 (88%)	132 (98%)	2 (2%)	57	81
1	T	133/153 (87%)	131 (98%)	2 (2%)	57	81
All	All	2678/3060 (88%)	2638 (98%)	40 (2%)	59	81

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	26	LYS
1	B	4	ASN
1	B	59[A]	GLU
1	B	59[B]	GLU
1	C	118[A]	ASP
1	C	118[B]	ASP
1	C	145	SER
1	D	58	GLU
1	D	86	GLU
1	D	148	LEU
1	E	150	LYS
1	F	26	LYS
1	F	145	SER
1	G	59	GLU
1	H	86	GLU
1	I	45	VAL
1	J	46[A]	CYS
1	J	46[B]	CYS

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Mol	Chain	Res	Type
1	K	26	LYS
1	K	29	GLU
1	K	45	VAL
1	K	62	LYS
1	L	138	GLU
1	M	26	LYS
1	M	92	LYS
1	N	45	VAL
1	N	145	SER
1	O	59	GLU
1	O	63	LEU
1	O	71	SER
1	O	148	LEU
1	P	145	SER
1	Q	130	ILE
1	R	26	LYS
1	R	86	GLU
1	S	138	GLU
1	S	148	LEU
1	T	1	SER
1	T	138	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	56	HIS
1	B	160	HIS
1	C	4	ASN
1	D	13	GLN
1	D	160	HIS
1	E	160	HIS
1	F	17	ASN
1	G	56	HIS
1	G	61	GLN
1	H	17	ASN
1	L	12	ASN
1	L	78	HIS
1	M	56	HIS
1	M	61	GLN
1	N	12	ASN
1	P	61	GLN
1	Q	12	ASN

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Mol	Chain	Res	Type
1	T	12	ASN
1	T	56	HIS
1	T	160	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 27 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

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	160/186 (86%)	-0.09	4 (2%) 58 55	26, 44, 72, 107	0
1	B	162/186 (87%)	-0.01	6 (3%) 45 41	26, 45, 80, 120	1 (0%)
1	C	162/186 (87%)	-0.14	5 (3%) 51 48	22, 37, 73, 134	1 (0%)
1	D	161/186 (86%)	-0.17	4 (2%) 58 55	23, 38, 73, 134	0
1	E	160/186 (86%)	-0.22	3 (1%) 66 63	23, 34, 68, 129	1 (0%)
1	F	161/186 (86%)	-0.21	4 (2%) 58 55	23, 38, 70, 153	0
1	G	161/186 (86%)	-0.16	3 (1%) 66 63	23, 40, 74, 138	0
1	H	161/186 (86%)	-0.28	3 (1%) 66 63	22, 35, 69, 121	1 (0%)
1	I	161/186 (86%)	0.03	4 (2%) 58 55	24, 46, 79, 121	1 (0%)
1	J	161/186 (86%)	-0.31	6 (3%) 45 41	15, 35, 68, 122	2 (1%)
1	K	160/186 (86%)	0.23	6 (3%) 44 40	27, 50, 86, 119	0
1	L	162/186 (87%)	-0.04	6 (3%) 45 41	26, 44, 82, 114	0
1	M	161/186 (86%)	0.20	6 (3%) 45 41	26, 55, 89, 121	0
1	N	160/186 (86%)	-0.10	3 (1%) 66 63	24, 41, 73, 127	0
1	O	160/186 (86%)	0.12	6 (3%) 44 40	26, 47, 78, 113	0
1	P	160/186 (86%)	0.03	4 (2%) 58 55	29, 47, 83, 138	0
1	Q	161/186 (86%)	0.03	4 (2%) 58 55	29, 44, 77, 139	0
1	R	161/186 (86%)	0.22	4 (2%) 58 55	30, 56, 91, 150	0
1	S	161/186 (86%)	-0.09	6 (3%) 45 41	26, 40, 78, 140	0
1	T	160/186 (86%)	-0.22	2 (1%) 75 73	26, 39, 73, 108	0
All	All	3216/3720 (86%)	-0.06	89 (2%) 55 51	15, 43, 80, 153	7 (0%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	44	PHE	5.3
1	D	44	PHE	4.9
1	E	44	PHE	4.8
1	K	45	VAL	4.8
1	F	44	PHE	4.8
1	H	44	PHE	4.6
1	B	45	VAL	4.4
1	R	44	PHE	4.2
1	P	45	VAL	4.2
1	M	44	PHE	4.1
1	C	44	PHE	4.1
1	G	44	PHE	4.1
1	L	44	PHE	4.0
1	L	45	VAL	4.0
1	P	44	PHE	3.9
1	N	44	PHE	3.8
1	Q	44	PHE	3.8
1	T	138	GLU	3.7
1	D	46	CYS	3.7
1	H	45	VAL	3.7
1	D	161	PRO	3.6
1	A	45	VAL	3.6
1	I	45	VAL	3.5
1	J	44	PHE	3.5
1	S	146	ASP	3.4
1	S	44	PHE	3.4
1	F	46	CYS	3.3
1	P	46	CYS	3.2
1	D	45	VAL	3.2
1	A	44	PHE	3.1
1	S	45	VAL	3.1
1	P	134	GLU	3.0
1	E	138	GLU	3.0
1	O	44	PHE	3.0
1	N	45	VAL	2.9
1	O	30	GLY	2.9
1	R	45	VAL	2.9
1	Q	45	VAL	2.9
1	I	44	PHE	2.8
1	B	162	GLY	2.8
1	I	138	GLU	2.8
1	T	44	PHE	2.8
1	K	29	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	O	45	VAL	2.7
1	F	58	GLU	2.7
1	L	138	GLU	2.7
1	C	162	GLY	2.6
1	L	162	GLY	2.6
1	A	48	THR	2.5
1	R	138	GLU	2.5
1	H	46	CYS	2.5
1	N	139	GLY	2.5
1	B	46	CYS	2.4
1	J	46[A]	CYS	2.4
1	K	44	PHE	2.4
1	C	45	VAL	2.4
1	C	46	CYS	2.4
1	F	45	VAL	2.4
1	M	17	ASN	2.4
1	M	55	ASP	2.3
1	K	139	GLY	2.3
1	C	138	GLU	2.3
1	A	139	GLY	2.3
1	Q	17	ASN	2.2
1	S	139	GLY	2.2
1	E	58	GLU	2.2
1	S	46	CYS	2.2
1	G	138	GLU	2.1
1	J	138	GLU	2.1
1	G	46	CYS	2.1
1	M	53	VAL	2.1
1	O	26	LYS	2.1
1	M	46	CYS	2.1
1	K	17	ASN	2.1
1	J	139	GLY	2.1
1	R	146	ASP	2.1
1	K	58	GLU	2.1
1	J	45	VAL	2.1
1	B	138	GLU	2.1
1	L	58	GLU	2.1
1	J	47	PRO	2.1
1	B	139	GLY	2.1
1	M	139	GLY	2.1
1	O	59	GLU	2.0
1	I	61	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	L	46	CYS	2.0
1	O	65	VAL	2.0
1	S	143	ASP	2.0
1	Q	161	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 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($\text{\AA}^2$)	Q<0.9
2	CL	H	202	1/1	0.74	0.23	78,78,78,78	0
2	CL	R	202	1/1	0.79	0.16	75,75,75,75	0
2	CL	N	201	1/1	0.80	0.28	104,104,104,104	0
2	CL	S	201	1/1	0.83	0.21	73,73,73,73	0
2	CL	A	201	1/1	0.84	0.25	85,85,85,85	0
2	CL	K	201	1/1	0.85	0.22	90,90,90,90	0
2	CL	M	201	1/1	0.86	0.19	80,80,80,80	0
2	CL	K	202	1/1	0.86	0.21	83,83,83,83	0
2	CL	E	201	1/1	0.87	0.20	75,75,75,75	0
2	CL	J	201	1/1	0.88	0.12	65,65,65,65	0
2	CL	O	201	1/1	0.88	0.24	72,72,72,72	0
2	CL	L	202	1/1	0.88	0.16	78,78,78,78	0
2	CL	C	202	1/1	0.88	0.17	73,73,73,73	0
2	CL	A	202	1/1	0.90	0.12	65,65,65,65	0
2	CL	T	201	1/1	0.90	0.23	68,68,68,68	0
2	CL	C	201	1/1	0.91	0.13	71,71,71,71	0
2	CL	B	201	1/1	0.91	0.14	71,71,71,71	0
2	CL	G	201	1/1	0.92	0.12	67,67,67,67	0
2	CL	L	201	1/1	0.92	0.15	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	I	201	1/1	0.92	0.13	61,61,61,61	0
2	CL	R	201	1/1	0.93	0.16	89,89,89,89	0
2	CL	O	202	1/1	0.93	0.12	74,74,74,74	0
2	CL	D	201	1/1	0.94	0.12	67,67,67,67	0
2	CL	J	202	1/1	0.94	0.12	57,57,57,57	0
2	CL	F	201	1/1	0.95	0.12	68,68,68,68	0
2	CL	H	201	1/1	0.97	0.10	74,74,74,74	0
2	CL	P	201	1/1	0.97	0.10	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.