



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:45 AM UTC

PDB ID : 8TNF / pdb_00008tnf
Title : Crystal structure of sulfohexulose-1-phosphate aldolase from *Paracoccus onubensis* strain Merri
Authors : Lee, M.
Deposited on : 2023-08-01
Resolution : 2.50 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:

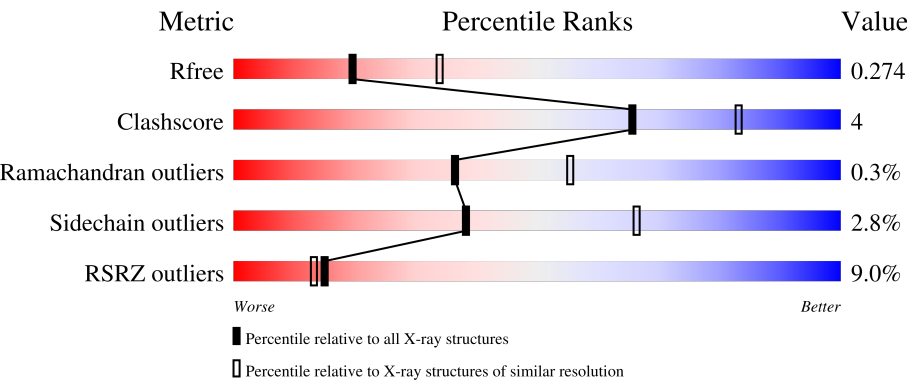
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	362	7% 82% 10% 8%
1	B	362	5% 82% 11% 7%
1	C	362	4% 82% 9% 8%
1	D	362	5% 78% 13% 8%
1	E	362	11% 81% 10% 9%

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Mol	Chain	Length	Quality of chain
1	F	362	7% 79% 11% 8%
1	G	362	11% 79% 12% 9%
1	H	362	17% 81% 9% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21084 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 DUF2090 domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2586	1637	457	483	9			
1	B	338	Total	C	N	O	S	0	0	0
			2615	1654	461	491	9			
1	C	332	Total	C	N	O	S	0	0	0
			2573	1630	455	479	9			
1	D	334	Total	C	N	O	S	0	0	0
			2577	1631	456	482	8			
1	E	331	Total	C	N	O	S	0	0	0
			2556	1618	451	478	9			
1	F	332	Total	C	N	O	S	0	0	0
			2573	1630	455	479	9			
1	G	331	Total	C	N	O	S	0	0	0
			2568	1627	454	478	9			
1	H	331	Total	C	N	O	S	0	0	0
			2552	1618	450	475	9			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	expression tag	UNP A0A418T8G4
A	-15	GLY	-	expression tag	UNP A0A418T8G4
A	-14	SER	-	expression tag	UNP A0A418T8G4
A	-13	SER	-	expression tag	UNP A0A418T8G4
A	-12	HIS	-	expression tag	UNP A0A418T8G4
A	-11	HIS	-	expression tag	UNP A0A418T8G4
A	-10	HIS	-	expression tag	UNP A0A418T8G4
A	-9	HIS	-	expression tag	UNP A0A418T8G4
A	-8	HIS	-	expression tag	UNP A0A418T8G4
A	-7	HIS	-	expression tag	UNP A0A418T8G4
A	-6	GLU	-	expression tag	UNP A0A418T8G4
A	-5	ASN	-	expression tag	UNP A0A418T8G4
A	-4	LEU	-	expression tag	UNP A0A418T8G4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	TYR	-	expression tag	UNP A0A418T8G4
A	-2	PHE	-	expression tag	UNP A0A418T8G4
A	-1	GLN	-	expression tag	UNP A0A418T8G4
A	0	GLY	-	expression tag	UNP A0A418T8G4
A	47	GLU	LYS	conflict	UNP A0A418T8G4
A	240	VAL	LEU	conflict	UNP A0A418T8G4
A	297	GLU	ASP	conflict	UNP A0A418T8G4
B	-16	MET	-	expression tag	UNP A0A418T8G4
B	-15	GLY	-	expression tag	UNP A0A418T8G4
B	-14	SER	-	expression tag	UNP A0A418T8G4
B	-13	SER	-	expression tag	UNP A0A418T8G4
B	-12	HIS	-	expression tag	UNP A0A418T8G4
B	-11	HIS	-	expression tag	UNP A0A418T8G4
B	-10	HIS	-	expression tag	UNP A0A418T8G4
B	-9	HIS	-	expression tag	UNP A0A418T8G4
B	-8	HIS	-	expression tag	UNP A0A418T8G4
B	-7	HIS	-	expression tag	UNP A0A418T8G4
B	-6	GLU	-	expression tag	UNP A0A418T8G4
B	-5	ASN	-	expression tag	UNP A0A418T8G4
B	-4	LEU	-	expression tag	UNP A0A418T8G4
B	-3	TYR	-	expression tag	UNP A0A418T8G4
B	-2	PHE	-	expression tag	UNP A0A418T8G4
B	-1	GLN	-	expression tag	UNP A0A418T8G4
B	0	GLY	-	expression tag	UNP A0A418T8G4
B	47	GLU	LYS	conflict	UNP A0A418T8G4
B	240	VAL	LEU	conflict	UNP A0A418T8G4
B	297	GLU	ASP	conflict	UNP A0A418T8G4
C	-16	MET	-	expression tag	UNP A0A418T8G4
C	-15	GLY	-	expression tag	UNP A0A418T8G4
C	-14	SER	-	expression tag	UNP A0A418T8G4
C	-13	SER	-	expression tag	UNP A0A418T8G4
C	-12	HIS	-	expression tag	UNP A0A418T8G4
C	-11	HIS	-	expression tag	UNP A0A418T8G4
C	-10	HIS	-	expression tag	UNP A0A418T8G4
C	-9	HIS	-	expression tag	UNP A0A418T8G4
C	-8	HIS	-	expression tag	UNP A0A418T8G4
C	-7	HIS	-	expression tag	UNP A0A418T8G4
C	-6	GLU	-	expression tag	UNP A0A418T8G4
C	-5	ASN	-	expression tag	UNP A0A418T8G4
C	-4	LEU	-	expression tag	UNP A0A418T8G4
C	-3	TYR	-	expression tag	UNP A0A418T8G4
C	-2	PHE	-	expression tag	UNP A0A418T8G4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLN	-	expression tag	UNP A0A418T8G4
C	0	GLY	-	expression tag	UNP A0A418T8G4
C	47	GLU	LYS	conflict	UNP A0A418T8G4
C	240	VAL	LEU	conflict	UNP A0A418T8G4
C	297	GLU	ASP	conflict	UNP A0A418T8G4
D	-16	MET	-	expression tag	UNP A0A418T8G4
D	-15	GLY	-	expression tag	UNP A0A418T8G4
D	-14	SER	-	expression tag	UNP A0A418T8G4
D	-13	SER	-	expression tag	UNP A0A418T8G4
D	-12	HIS	-	expression tag	UNP A0A418T8G4
D	-11	HIS	-	expression tag	UNP A0A418T8G4
D	-10	HIS	-	expression tag	UNP A0A418T8G4
D	-9	HIS	-	expression tag	UNP A0A418T8G4
D	-8	HIS	-	expression tag	UNP A0A418T8G4
D	-7	HIS	-	expression tag	UNP A0A418T8G4
D	-6	GLU	-	expression tag	UNP A0A418T8G4
D	-5	ASN	-	expression tag	UNP A0A418T8G4
D	-4	LEU	-	expression tag	UNP A0A418T8G4
D	-3	TYR	-	expression tag	UNP A0A418T8G4
D	-2	PHE	-	expression tag	UNP A0A418T8G4
D	-1	GLN	-	expression tag	UNP A0A418T8G4
D	0	GLY	-	expression tag	UNP A0A418T8G4
D	47	GLU	LYS	conflict	UNP A0A418T8G4
D	240	VAL	LEU	conflict	UNP A0A418T8G4
D	297	GLU	ASP	conflict	UNP A0A418T8G4
E	-16	MET	-	expression tag	UNP A0A418T8G4
E	-15	GLY	-	expression tag	UNP A0A418T8G4
E	-14	SER	-	expression tag	UNP A0A418T8G4
E	-13	SER	-	expression tag	UNP A0A418T8G4
E	-12	HIS	-	expression tag	UNP A0A418T8G4
E	-11	HIS	-	expression tag	UNP A0A418T8G4
E	-10	HIS	-	expression tag	UNP A0A418T8G4
E	-9	HIS	-	expression tag	UNP A0A418T8G4
E	-8	HIS	-	expression tag	UNP A0A418T8G4
E	-7	HIS	-	expression tag	UNP A0A418T8G4
E	-6	GLU	-	expression tag	UNP A0A418T8G4
E	-5	ASN	-	expression tag	UNP A0A418T8G4
E	-4	LEU	-	expression tag	UNP A0A418T8G4
E	-3	TYR	-	expression tag	UNP A0A418T8G4
E	-2	PHE	-	expression tag	UNP A0A418T8G4
E	-1	GLN	-	expression tag	UNP A0A418T8G4
E	0	GLY	-	expression tag	UNP A0A418T8G4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	47	GLU	LYS	conflict	UNP A0A418T8G4
E	240	VAL	LEU	conflict	UNP A0A418T8G4
E	297	GLU	ASP	conflict	UNP A0A418T8G4
F	-16	MET	-	expression tag	UNP A0A418T8G4
F	-15	GLY	-	expression tag	UNP A0A418T8G4
F	-14	SER	-	expression tag	UNP A0A418T8G4
F	-13	SER	-	expression tag	UNP A0A418T8G4
F	-12	HIS	-	expression tag	UNP A0A418T8G4
F	-11	HIS	-	expression tag	UNP A0A418T8G4
F	-10	HIS	-	expression tag	UNP A0A418T8G4
F	-9	HIS	-	expression tag	UNP A0A418T8G4
F	-8	HIS	-	expression tag	UNP A0A418T8G4
F	-7	HIS	-	expression tag	UNP A0A418T8G4
F	-6	GLU	-	expression tag	UNP A0A418T8G4
F	-5	ASN	-	expression tag	UNP A0A418T8G4
F	-4	LEU	-	expression tag	UNP A0A418T8G4
F	-3	TYR	-	expression tag	UNP A0A418T8G4
F	-2	PHE	-	expression tag	UNP A0A418T8G4
F	-1	GLN	-	expression tag	UNP A0A418T8G4
F	0	GLY	-	expression tag	UNP A0A418T8G4
F	47	GLU	LYS	conflict	UNP A0A418T8G4
F	240	VAL	LEU	conflict	UNP A0A418T8G4
F	297	GLU	ASP	conflict	UNP A0A418T8G4
G	-16	MET	-	expression tag	UNP A0A418T8G4
G	-15	GLY	-	expression tag	UNP A0A418T8G4
G	-14	SER	-	expression tag	UNP A0A418T8G4
G	-13	SER	-	expression tag	UNP A0A418T8G4
G	-12	HIS	-	expression tag	UNP A0A418T8G4
G	-11	HIS	-	expression tag	UNP A0A418T8G4
G	-10	HIS	-	expression tag	UNP A0A418T8G4
G	-9	HIS	-	expression tag	UNP A0A418T8G4
G	-8	HIS	-	expression tag	UNP A0A418T8G4
G	-7	HIS	-	expression tag	UNP A0A418T8G4
G	-6	GLU	-	expression tag	UNP A0A418T8G4
G	-5	ASN	-	expression tag	UNP A0A418T8G4
G	-4	LEU	-	expression tag	UNP A0A418T8G4
G	-3	TYR	-	expression tag	UNP A0A418T8G4
G	-2	PHE	-	expression tag	UNP A0A418T8G4
G	-1	GLN	-	expression tag	UNP A0A418T8G4
G	0	GLY	-	expression tag	UNP A0A418T8G4
G	47	GLU	LYS	conflict	UNP A0A418T8G4
G	240	VAL	LEU	conflict	UNP A0A418T8G4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	297	GLU	ASP	conflict	UNP A0A418T8G4
H	-16	MET	-	expression tag	UNP A0A418T8G4
H	-15	GLY	-	expression tag	UNP A0A418T8G4
H	-14	SER	-	expression tag	UNP A0A418T8G4
H	-13	SER	-	expression tag	UNP A0A418T8G4
H	-12	HIS	-	expression tag	UNP A0A418T8G4
H	-11	HIS	-	expression tag	UNP A0A418T8G4
H	-10	HIS	-	expression tag	UNP A0A418T8G4
H	-9	HIS	-	expression tag	UNP A0A418T8G4
H	-8	HIS	-	expression tag	UNP A0A418T8G4
H	-7	HIS	-	expression tag	UNP A0A418T8G4
H	-6	GLU	-	expression tag	UNP A0A418T8G4
H	-5	ASN	-	expression tag	UNP A0A418T8G4
H	-4	LEU	-	expression tag	UNP A0A418T8G4
H	-3	TYR	-	expression tag	UNP A0A418T8G4
H	-2	PHE	-	expression tag	UNP A0A418T8G4
H	-1	GLN	-	expression tag	UNP A0A418T8G4
H	0	GLY	-	expression tag	UNP A0A418T8G4
H	47	GLU	LYS	conflict	UNP A0A418T8G4
H	240	VAL	LEU	conflict	UNP A0A418T8G4
H	297	GLU	ASP	conflict	UNP A0A418T8G4

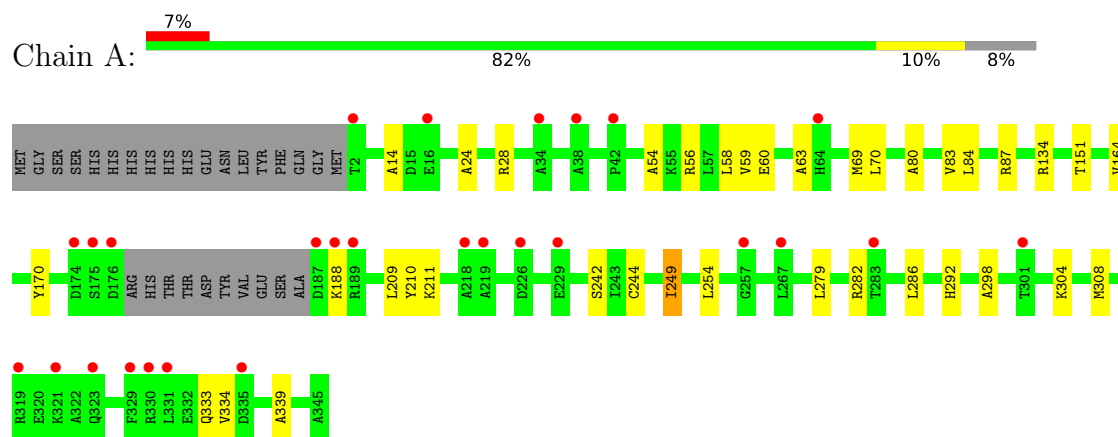
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	59	Total O 59 59	0	0
2	B	57	Total O 57 57	0	0
2	C	77	Total O 77 77	0	0
2	D	86	Total O 86 86	0	0
2	E	56	Total O 56 56	0	0
2	F	65	Total O 65 65	0	0
2	G	45	Total O 45 45	0	0
2	H	39	Total O 39 39	0	0

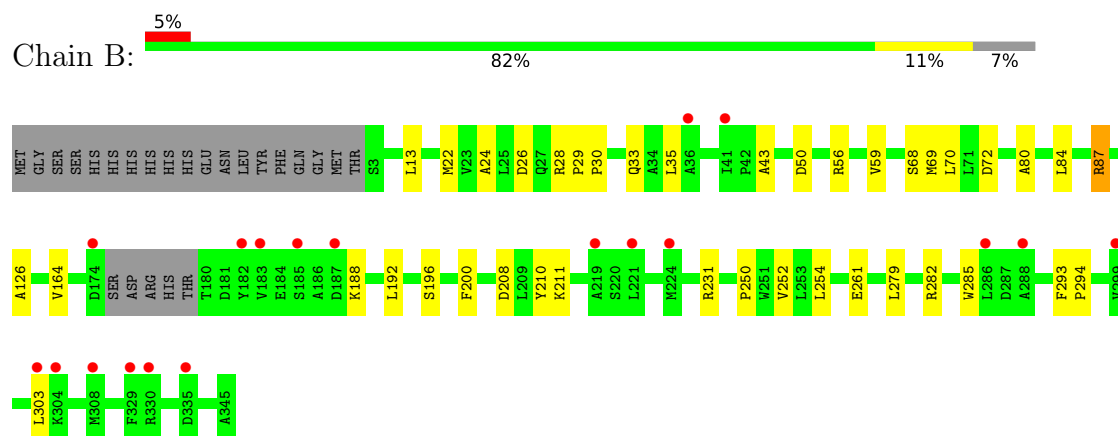
3 Residue-property plots [i](#)

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.

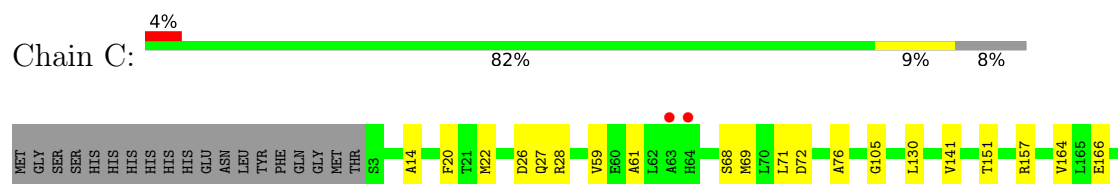
- Molecule 1: DUF2090 domain-containing protein

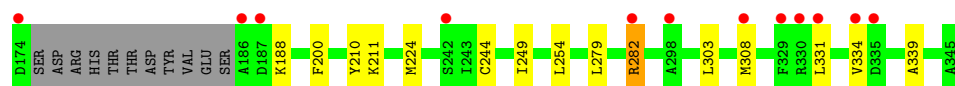


- Molecule 1: DUF2090 domain-containing protein

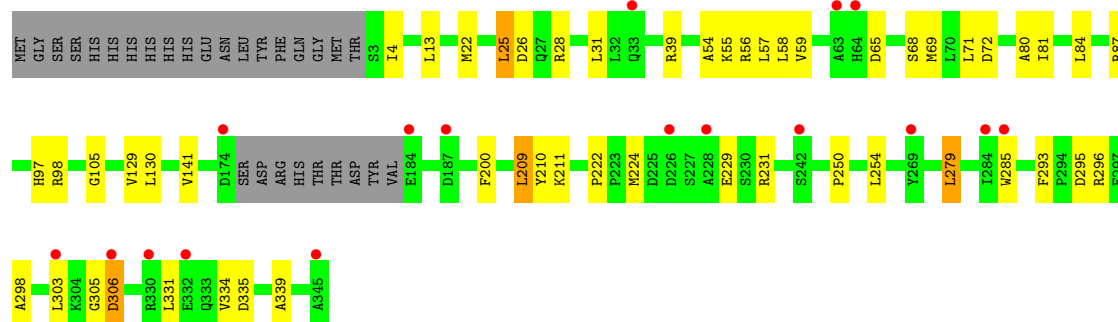
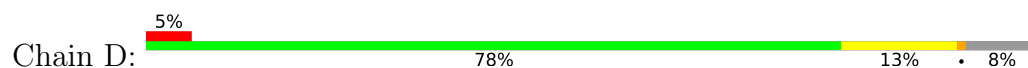


- Molecule 1: DUF2090 domain-containing protein

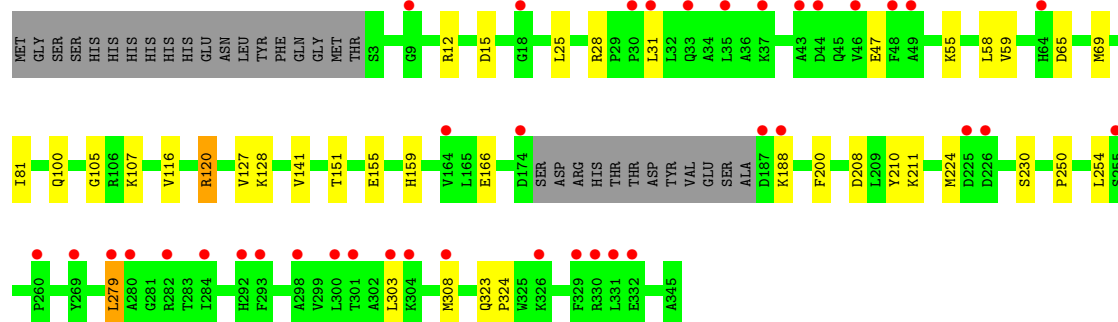
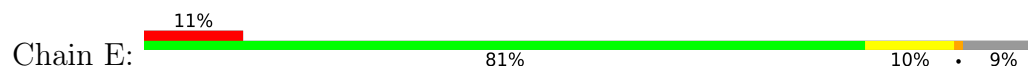




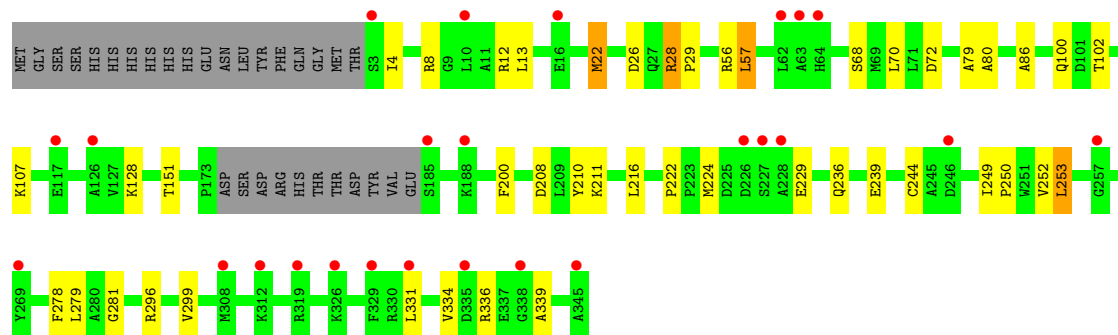
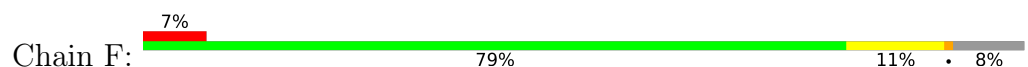
- Molecule 1: DUF2090 domain-containing protein



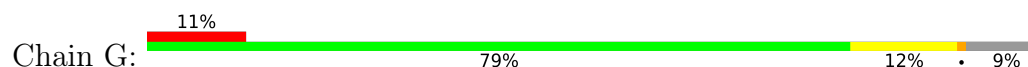
- Molecule 1: DUF2090 domain-containing protein

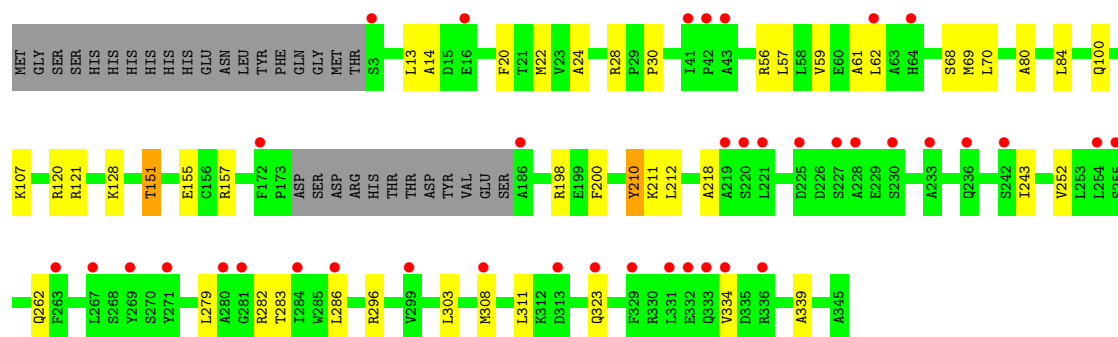


- Molecule 1: DUF2090 domain-containing protein

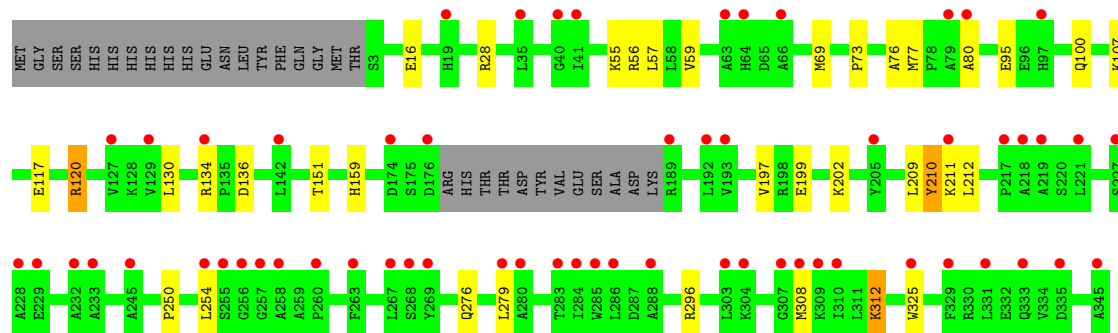
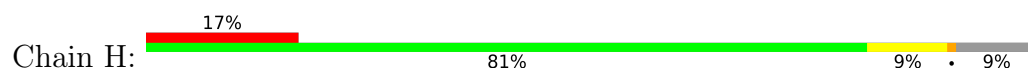


- Molecule 1: DUF2090 domain-containing protein





• Molecule 1: DUF2090 domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	78.66Å 82.48Å 144.77Å 96.05° 90.00° 97.42°	Depositor
Resolution (Å)	47.88 – 2.50 47.88 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.7 (47.88-2.50) 97.7 (47.88-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.237 , 0.282 0.230 , 0.274	Depositor DCC
R_{free} test set	6050 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21084	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.83% 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

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	0.69	0/2642	1.07	5/3583 (0.1%)
1	B	0.66	0/2671	1.07	3/3623 (0.1%)
1	C	0.70	0/2629	1.07	1/3565 (0.0%)
1	D	0.74	0/2633	1.07	4/3573 (0.1%)
1	E	0.68	0/2611	1.07	2/3542 (0.1%)
1	F	0.71	1/2629 (0.0%)	1.06	4/3565 (0.1%)
1	G	0.63	0/2624	1.06	1/3558 (0.0%)
1	H	0.63	0/2608	1.05	0/3539
All	All	0.68	1/21047 (0.0%)	1.06	20/28548 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	22	MET	SD-CE	-5.29	1.66	1.79

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	200	PHE	CA-CB-CG	-6.31	107.49	113.80
1	E	200	PHE	CA-CB-CG	-6.08	107.72	113.80
1	F	281	GLY	CA-C-N	6.01	129.83	120.82
1	F	281	GLY	C-N-CA	6.01	129.83	120.82
1	A	249	ILE	N-CA-C	5.94	113.43	107.55
1	F	200	PHE	CA-CB-CG	-5.76	108.03	113.80
1	D	305	GLY	CA-C-N	5.70	127.85	120.44
1	D	305	GLY	C-N-CA	5.70	127.85	120.44
1	B	200	PHE	CA-CB-CG	-5.66	108.14	113.80
1	G	200	PHE	CA-CB-CG	-5.63	108.17	113.80
1	D	200	PHE	CA-CB-CG	-5.62	108.18	113.80
1	E	15	ASP	CA-CB-CG	5.61	118.21	112.60
1	F	79	ALA	N-CA-C	5.46	117.31	111.36
1	A	333	GLN	CA-C-N	5.25	129.70	123.19
1	A	333	GLN	C-N-CA	5.25	129.70	123.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	43	ALA	CA-C-N	5.13	128.80	120.60
1	B	43	ALA	C-N-CA	5.13	128.80	120.60
1	D	306	ASP	N-CA-C	5.11	116.53	111.07
1	A	188	LYS	CA-C-N	5.03	127.01	120.28
1	A	188	LYS	C-N-CA	5.03	127.01	120.28

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	2586	0	2563	19	0
1	B	2615	0	2587	24	0
1	C	2573	0	2554	18	0
1	D	2577	0	2543	28	0
1	E	2556	0	2531	16	0
1	F	2573	0	2554	22	0
1	G	2568	0	2552	22	0
1	H	2552	0	2524	16	0
2	A	59	0	0	0	0
2	B	57	0	0	0	0
2	C	77	0	0	0	0
2	D	86	0	0	0	0
2	E	56	0	0	1	0
2	F	65	0	0	0	0
2	G	45	0	0	0	0
2	H	39	0	0	0	0
All	All	21084	0	20408	157	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 (157) 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:D:211:LYS:CE	1:D:279:LEU:HG	2.03	0.89
1:D:211:LYS:HE3	1:D:279:LEU:HG	1.56	0.87
1:A:87:ARG:HG3	1:B:87:ARG:HG2	1.61	0.82
1:G:30:PRO:HB3	1:G:282:ARG:HD3	1.63	0.81
1:A:334:VAL:HG13	1:A:339:ALA:HB3	1.64	0.77
1:A:87:ARG:HG3	1:B:87:ARG:CG	2.18	0.72
1:B:30:PRO:HB3	1:B:282:ARG:HD3	1.73	0.71
1:A:282:ARG:HE	1:A:286:LEU:HD13	1.58	0.69
1:D:211:LYS:HE2	1:D:279:LEU:HG	1.75	0.68
1:H:57:LEU:HD21	1:H:296:ARG:HG3	1.78	0.66
1:D:59:VAL:HG13	1:D:69:MET:HE1	1.78	0.65
1:D:334:VAL:HG13	1:D:339:ALA:HB3	1.78	0.65
1:E:211:LYS:HE3	1:E:279:LEU:HG	1.78	0.65
1:E:31:LEU:HD23	1:E:55:LYS:HE2	1.80	0.64
1:D:57:LEU:HD21	1:D:296:ARG:HG3	1.79	0.63
1:H:134:ARG:HB3	1:H:136:ASP:OD1	1.99	0.61
1:A:211:LYS:HD3	1:A:279:LEU:HD22	1.82	0.61
1:C:282:ARG:HE	1:C:282:ARG:H	1.46	0.61
1:A:292:HIS:ND1	1:A:298:ALA:HB1	2.16	0.61
1:H:55:LYS:HD3	1:H:76:ALA:HB2	1.83	0.61
1:B:211:LYS:HD3	1:B:279:LEU:HD22	1.81	0.60
1:B:164:VAL:HG11	1:B:211:LYS:HE3	1.84	0.60
1:G:303:LEU:HB3	1:G:308:MET:HE3	1.84	0.60
1:G:334:VAL:HG13	1:G:339:ALA:HB3	1.85	0.59
1:A:304:LYS:HA	1:A:308:MET:HG3	1.83	0.59
1:D:25:LEU:HD21	1:D:69:MET:HE3	1.84	0.58
1:C:20:PHE:HB3	1:C:22:MET:HE3	1.87	0.57
1:B:69:MET:HE2	1:B:84:LEU:HD13	1.86	0.57
1:A:87:ARG:CG	1:B:87:ARG:HG2	2.35	0.57
1:C:211:LYS:HD3	1:C:279:LEU:HD22	1.85	0.57
1:H:95:GLU:HG2	1:H:130:LEU:H	1.70	0.56
1:G:24:ALA:HA	1:G:70:LEU:HB3	1.89	0.54
1:A:56:ARG:HA	1:A:80:ALA:HB2	1.90	0.54
1:D:4:ILE:HD11	1:D:331:LEU:HD21	1.89	0.54
1:C:244:CYS:HB3	1:C:249:ILE:O	2.08	0.53
1:C:334:VAL:HG13	1:C:339:ALA:HB3	1.89	0.53
1:F:222:PRO:HG3	1:F:229:GLU:HG2	1.90	0.53
1:F:22:MET:CE	1:F:252:VAL:HG21	2.39	0.53
1:D:25:LEU:HD11	1:D:71:LEU:HD22	1.89	0.53
1:B:208:ASP:O	1:B:250:PRO:HD2	2.10	0.52
1:C:27:GLN:HE21	1:C:282:ARG:NE	2.07	0.52
1:G:70:LEU:HD11	1:G:128:LYS:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:ARG:H	1:C:282:ARG:NE	2.06	0.52
1:D:31:LEU:HD22	1:D:55:LYS:HE2	1.91	0.52
1:F:4:ILE:HD11	1:F:331:LEU:HD21	1.92	0.51
1:D:39:ARG:HH11	1:D:293:PHE:HE2	1.59	0.50
1:E:116:VAL:HG22	1:E:127:VAL:HG11	1.93	0.50
1:F:253:LEU:H	1:F:278:PHE:HA	1.76	0.50
1:A:69:MET:HE2	1:A:84:LEU:HD13	1.94	0.50
1:C:61:ALA:HB1	1:C:308:MET:HE2	1.93	0.50
1:C:59:VAL:HG13	1:C:69:MET:HE1	1.92	0.50
1:C:14:ALA:O	1:D:87:ARG:NH2	2.45	0.50
1:F:57:LEU:HD21	1:F:296:ARG:HG3	1.94	0.50
1:B:29:PRO:O	1:B:33:GLN:HG2	2.12	0.50
1:D:97:HIS:CE1	1:D:98:ARG:NH1	2.80	0.49
1:A:59:VAL:HG22	1:A:69:MET:HE1	1.95	0.49
1:A:14:ALA:O	1:B:87:ARG:NH2	2.45	0.49
1:E:323:GLN:HG2	1:E:324:PRO:HD2	1.94	0.49
1:E:65:ASP:OD2	1:E:308:MET:SD	2.71	0.49
1:G:13:LEU:HA	1:G:68:SER:HB3	1.94	0.49
1:F:28:ARG:HB2	1:F:29:PRO:HD3	1.94	0.49
1:G:69:MET:HE2	1:G:84:LEU:HD13	1.94	0.49
1:A:24:ALA:HA	1:A:70:LEU:HB3	1.94	0.49
1:F:211:LYS:HD3	1:F:279:LEU:HD22	1.94	0.49
1:A:134:ARG:HD2	1:A:170:TYR:O	2.13	0.49
1:D:105:GLY:HA3	1:D:141:VAL:HG11	1.95	0.49
1:F:100:GLN:HB3	1:F:107:LYS:HB2	1.93	0.48
1:G:210:TYR:HB3	1:G:212:LEU:HG	1.95	0.48
1:H:209:LEU:HD12	1:H:250:PRO:HG2	1.95	0.48
1:B:22:MET:HE1	1:B:252:VAL:HG21	1.96	0.48
1:C:71:LEU:HD22	1:C:76:ALA:HB1	1.95	0.48
1:H:308:MET:O	1:H:312:LYS:HD3	2.14	0.48
1:A:59:VAL:O	1:A:63:ALA:HB2	2.14	0.47
1:D:22:MET:HE3	1:D:279:LEU:HD23	1.95	0.47
1:G:282:ARG:HB3	1:G:286:LEU:HD22	1.95	0.47
1:G:151:THR:O	1:G:155:GLU:HG2	2.15	0.47
1:H:199:GLU:HA	1:H:202:LYS:HE3	1.96	0.47
1:B:22:MET:CE	1:B:252:VAL:HG21	2.45	0.47
1:F:13:LEU:HA	1:F:68:SER:HB3	1.97	0.46
1:D:39:ARG:NH1	1:D:293:PHE:CE2	2.83	0.46
1:B:13:LEU:HA	1:B:68:SER:HB3	1.98	0.46
1:D:295:ASP:HB3	1:D:298:ALA:HB3	1.96	0.46
1:H:59:VAL:HA	1:H:69:MET:HE1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:211:LYS:HE2	1:H:279:LEU:HD13	1.98	0.46
1:F:26:ASP:HB2	1:F:72:ASP:HB3	1.98	0.46
1:D:69:MET:HE2	1:D:84:LEU:HD13	1.98	0.46
1:E:59:VAL:HG13	1:E:69:MET:HE1	1.98	0.46
1:C:282:ARG:HE	1:C:282:ARG:N	2.12	0.46
1:E:100:GLN:HB3	1:E:107:LYS:HB2	1.98	0.46
1:G:61:ALA:HB1	1:G:308:MET:HE2	1.97	0.46
1:G:100:GLN:HB2	1:G:107:LYS:HB2	1.97	0.45
1:H:100:GLN:HB3	1:H:107:LYS:HB2	1.99	0.45
1:A:164:VAL:HG22	1:A:209:LEU:HB3	1.97	0.45
1:B:35:LEU:HD13	1:B:50:ASP:HB3	1.98	0.45
1:C:130:LEU:HA	1:C:166:GLU:HB3	1.98	0.45
1:B:285:TRP:HB3	1:B:303:LEU:HD21	1.99	0.45
1:G:218:ALA:HB1	1:G:262:GLN:HB3	1.98	0.45
1:H:210:TYR:HB3	1:H:212:LEU:HG	1.98	0.45
1:B:59:VAL:HG22	1:B:69:MET:HE1	1.97	0.45
1:F:56:ARG:HA	1:F:80:ALA:HB2	1.98	0.45
1:G:14:ALA:HB2	1:G:20:PHE:CE1	2.51	0.45
1:G:22:MET:HE2	1:G:252:VAL:HG21	1.98	0.45
1:D:58:LEU:HD23	1:D:303:LEU:HD11	1.98	0.45
1:D:231:ARG:HD2	1:F:239:GLU:HB2	1.98	0.45
1:E:81:ILE:HD11	1:F:8:ARG:HD2	1.99	0.45
1:G:62:LEU:HD22	1:G:311:LEU:HD22	1.99	0.45
1:B:24:ALA:HA	1:B:70:LEU:HB3	1.99	0.44
1:E:128:LYS:NZ	2:E:403:HOH:O	2.50	0.44
1:C:303:LEU:HB3	1:C:308:MET:HE3	1.98	0.44
1:F:244:CYS:HB3	1:F:249:ILE:O	2.18	0.44
1:H:197:VAL:HG22	1:H:212:LEU:HD22	1.98	0.44
1:H:120:ARG:HG2	1:H:159:HIS:HB3	2.00	0.44
1:F:8:ARG:HH21	1:F:12:ARG:NH2	2.15	0.44
1:E:12:ARG:HG3	1:F:86:ALA:HB1	1.99	0.44
1:A:244:CYS:HB3	1:A:249:ILE:O	2.18	0.44
1:C:26:ASP:HB2	1:C:72:ASP:HB3	1.99	0.44
1:H:73:PRO:HA	1:H:77:MET:CG	2.48	0.44
1:B:13:LEU:HD11	1:B:126:ALA:HB2	2.00	0.44
1:G:211:LYS:HE2	1:G:279:LEU:HD13	2.00	0.44
1:E:151:THR:O	1:E:155:GLU:HG2	2.18	0.43
1:E:166:GLU:HB2	1:E:211:LYS:HD3	2.00	0.43
1:H:276:GLN:HG2	1:H:325:TRP:HB2	2.00	0.43
1:C:22:MET:HG2	1:C:68:SER:OG	2.18	0.43
1:A:54:ALA:O	1:A:58:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:LYS:HB3	1:B:254:LEU:HD21	2.00	0.43
1:D:26:ASP:HB2	1:D:72:ASP:HB3	2.00	0.43
1:D:54:ALA:O	1:D:58:LEU:HG	2.19	0.43
1:C:164:VAL:HG11	1:C:211:LYS:HE3	2.00	0.43
1:E:105:GLY:HA3	1:E:141:VAL:HG11	2.01	0.43
1:G:198:ARG:HA	1:G:243:ILE:HG21	2.01	0.42
1:E:208:ASP:O	1:E:250:PRO:HD2	2.19	0.42
1:D:222:PRO:HG3	1:D:229:GLU:HG2	2.01	0.42
1:B:56:ARG:HA	1:B:80:ALA:HB2	2.02	0.42
1:F:70:LEU:HD11	1:F:128:LYS:HD2	2.02	0.42
1:D:13:LEU:HA	1:D:68:SER:HB2	2.01	0.42
1:A:60:GLU:HG3	1:A:83:VAL:HG21	2.00	0.42
1:B:293:PHE:CG	1:B:294:PRO:HA	2.55	0.42
1:B:26:ASP:HB2	1:B:72:ASP:HB3	2.01	0.42
1:B:192:LEU:O	1:B:196:SER:OG	2.33	0.42
1:G:57:LEU:HD13	1:G:296:ARG:HG3	2.01	0.42
1:B:293:PHE:CD1	1:B:294:PRO:HA	2.55	0.41
1:F:22:MET:HG2	1:F:68:SER:OG	2.20	0.41
1:G:56:ARG:HA	1:G:80:ALA:HB2	2.02	0.41
1:D:81:ILE:HD12	1:D:81:ILE:HA	1.98	0.41
1:D:285:TRP:HB3	1:D:303:LEU:HD21	2.02	0.41
1:F:216:LEU:HD21	1:F:236:GLN:HG3	2.02	0.41
1:D:56:ARG:HA	1:D:80:ALA:HB2	2.02	0.41
1:G:22:MET:CE	1:G:252:VAL:HG21	2.50	0.41
1:F:57:LEU:HD13	1:F:299:VAL:HG11	2.02	0.41
1:G:59:VAL:HG22	1:G:69:MET:HE1	2.01	0.41
1:E:120:ARG:HG3	1:E:159:HIS:HB3	2.01	0.41
1:D:209:LEU:HD12	1:D:250:PRO:HG2	2.03	0.41
1:F:336:ARG:HG3	1:F:339:ALA:HB2	2.02	0.40
1:H:56:ARG:HA	1:H:80:ALA:HB2	2.02	0.40
1:C:105:GLY:HA3	1:C:141:VAL:HG11	2.03	0.40
1:E:58:LEU:HD23	1:E:303:LEU:HD11	2.04	0.40
1:F:208:ASP:O	1:F:250:PRO:HD2	2.20	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	330/362 (91%)	322 (98%)	7 (2%)	1 (0%)	36	55
1	B	334/362 (92%)	325 (97%)	8 (2%)	1 (0%)	36	55
1	C	328/362 (91%)	318 (97%)	9 (3%)	1 (0%)	36	55
1	D	330/362 (91%)	321 (97%)	8 (2%)	1 (0%)	36	55
1	E	327/362 (90%)	321 (98%)	5 (2%)	1 (0%)	36	55
1	F	328/362 (91%)	317 (97%)	10 (3%)	1 (0%)	36	55
1	G	327/362 (90%)	321 (98%)	5 (2%)	1 (0%)	36	55
1	H	327/362 (90%)	316 (97%)	10 (3%)	1 (0%)	36	55
All	All	2631/2896 (91%)	2561 (97%)	62 (2%)	8 (0%)	36	55

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	28	ARG
1	A	28	ARG
1	E	28	ARG
1	H	28	ARG
1	B	28	ARG
1	C	28	ARG
1	D	28	ARG
1	F	28	ARG

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	264/291 (91%)	260 (98%)	4 (2%)	57	80
1	B	267/291 (92%)	262 (98%)	5 (2%)	50	76
1	C	262/291 (90%)	254 (97%)	8 (3%)	35	62
1	D	261/291 (90%)	250 (96%)	11 (4%)	26	52
1	E	260/291 (89%)	251 (96%)	9 (4%)	32	58
1	F	262/291 (90%)	255 (97%)	7 (3%)	39	67
1	G	262/291 (90%)	255 (97%)	7 (3%)	39	67
1	H	259/291 (89%)	252 (97%)	7 (3%)	39	67
All	All	2097/2328 (90%)	2039 (97%)	58 (3%)	38	66

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	THR
1	A	210	TYR
1	A	242	SER
1	A	254	LEU
1	B	87	ARG
1	B	188	LYS
1	B	210	TYR
1	B	231	ARG
1	B	261	GLU
1	C	151	THR
1	C	157	ARG
1	C	188	LYS
1	C	210	TYR
1	C	224	MET
1	C	254	LEU
1	C	282	ARG
1	C	331	LEU
1	D	25	LEU
1	D	65	ASP
1	D	129	VAL
1	D	130	LEU
1	D	209	LEU
1	D	210	TYR
1	D	224	MET
1	D	254	LEU
1	D	279	LEU
1	D	306	ASP

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Mol	Chain	Res	Type
1	D	335	ASP
1	E	25	LEU
1	E	47	GLU
1	E	120	ARG
1	E	188	LYS
1	E	210	TYR
1	E	224	MET
1	E	230	SER
1	E	254	LEU
1	E	279	LEU
1	F	57	LEU
1	F	102	THR
1	F	151	THR
1	F	210	TYR
1	F	224	MET
1	F	253	LEU
1	F	334	VAL
1	G	120	ARG
1	G	121	ARG
1	G	151	THR
1	G	157	ARG
1	G	210	TYR
1	G	283	THR
1	G	323	GLN
1	H	16	GLU
1	H	117	GLU
1	H	120	ARG
1	H	151	THR
1	H	210	TYR
1	H	254	LEU
1	H	312	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	113	ASN
1	B	159	HIS
1	B	262	GLN
1	C	100	GLN
1	C	113	ASN
1	C	290	GLN

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Mol	Chain	Res	Type
1	C	292	HIS
1	C	333	GLN
1	D	45	GLN
1	D	113	ASN
1	D	276	GLN
1	F	276	GLN
1	G	113	ASN
1	G	292	HIS
1	H	19	HIS
1	H	290	GLN

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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/362 (92%)	0.77	27 (8%) 18 15	29, 49, 72, 84	0
1	B	338/362 (93%)	0.72	19 (5%) 30 26	31, 50, 76, 84	0
1	C	332/362 (91%)	0.58	14 (4%) 40 36	30, 44, 64, 80	0
1	D	334/362 (92%)	0.60	17 (5%) 33 29	28, 42, 67, 80	0
1	E	331/362 (91%)	1.00	39 (11%) 9 7	33, 50, 84, 94	0
1	F	332/362 (91%)	0.77	25 (7%) 20 18	34, 48, 68, 81	0
1	G	331/362 (91%)	1.01	39 (11%) 9 7	36, 55, 80, 91	0
1	H	331/362 (91%)	1.31	60 (18%) 3 3	38, 62, 86, 100	0
All	All	2663/2896 (91%)	0.84	240 (9%) 15 13	28, 50, 79, 100	0

All (240) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	345	ALA	5.2
1	E	37	LYS	4.9
1	E	174	ASP	4.7
1	A	176	ASP	4.7
1	H	245	ALA	4.4
1	H	267	LEU	4.2
1	H	176	ASP	4.1
1	H	189	ARG	4.1
1	E	308	MET	4.0
1	H	257	GLY	3.9
1	H	229	GLU	3.8
1	G	186	ALA	3.8
1	G	43	ALA	3.7
1	G	254	LEU	3.7
1	B	219	ALA	3.7
1	H	263	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	H	80	ALA	3.6
1	C	335	ASP	3.5
1	E	64	HIS	3.5
1	F	331	LEU	3.4
1	H	288	ALA	3.4
1	D	174	ASP	3.4
1	G	329	PHE	3.4
1	B	183	VAL	3.4
1	E	269	TYR	3.4
1	E	332	GLU	3.4
1	F	308	MET	3.3
1	A	16	GLU	3.3
1	F	338	GLY	3.3
1	B	182	TYR	3.3
1	H	308	MET	3.3
1	D	226	ASP	3.3
1	G	281	GLY	3.2
1	C	186	ALA	3.2
1	E	279	LEU	3.2
1	B	308	MET	3.2
1	G	269	TYR	3.1
1	G	242	SER	3.1
1	G	286	LEU	3.0
1	C	187	ASP	3.0
1	H	335	ASP	3.0
1	D	33	GLN	3.0
1	A	219	ALA	3.0
1	A	187	ASP	3.0
1	E	33	GLN	3.0
1	E	46	VAL	3.0
1	E	43	ALA	3.0
1	D	269	TYR	3.0
1	E	187	ASP	3.0
1	H	309	LYS	3.0
1	D	242	SER	3.0
1	A	2	THR	2.9
1	G	280	ALA	2.9
1	E	330	ARG	2.9
1	C	64	HIS	2.9
1	H	63	ALA	2.9
1	F	329	PHE	2.9
1	E	280	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	228	ALA	2.9
1	H	331	LEU	2.9
1	C	174	ASP	2.9
1	D	63	ALA	2.8
1	G	62	LEU	2.8
1	H	307	GLY	2.8
1	H	97	HIS	2.8
1	D	64	HIS	2.8
1	B	185	SER	2.7
1	H	286	LEU	2.7
1	E	225	ASP	2.7
1	H	256	GLY	2.7
1	E	331	LEU	2.7
1	H	283	THR	2.7
1	G	284	ILE	2.7
1	E	298	ALA	2.7
1	F	126	ALA	2.7
1	C	330	ARG	2.7
1	D	184	GLU	2.7
1	E	255	SER	2.6
1	H	325	TRP	2.6
1	H	41	ILE	2.6
1	H	329	PHE	2.6
1	B	303	LEU	2.6
1	G	299	VAL	2.6
1	G	255	SER	2.6
1	C	298	ALA	2.6
1	H	233	ALA	2.6
1	D	285	TRP	2.6
1	D	332	GLU	2.6
1	G	228	ALA	2.6
1	E	293	PHE	2.6
1	E	300	LEU	2.6
1	E	303	LEU	2.6
1	A	301	THR	2.6
1	E	304	LYS	2.6
1	A	267	LEU	2.5
1	G	267	LEU	2.5
1	H	279	LEU	2.5
1	F	345	ALA	2.5
1	H	258	ALA	2.5
1	B	174	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	299	VAL	2.5
1	A	38	ALA	2.5
1	E	282	ARG	2.5
1	B	187	ASP	2.5
1	E	226	ASP	2.5
1	G	332	GLU	2.5
1	A	331	LEU	2.5
1	H	221	LEU	2.5
1	B	304	LYS	2.5
1	D	345	ALA	2.5
1	F	226	ASP	2.5
1	F	335	ASP	2.5
1	G	221	LEU	2.5
1	A	283	THR	2.5
1	G	271	TYR	2.4
1	H	285	TRP	2.4
1	G	3	SER	2.4
1	G	220	SER	2.4
1	A	229	GLU	2.4
1	H	19	HIS	2.4
1	H	232	ALA	2.4
1	A	42	PRO	2.4
1	F	312	LYS	2.4
1	E	329	PHE	2.4
1	E	164	VAL	2.4
1	D	228	ALA	2.4
1	D	306	ASP	2.4
1	G	225	ASP	2.4
1	G	236	GLN	2.4
1	G	64	HIS	2.4
1	G	331	LEU	2.4
1	H	64	HIS	2.4
1	G	172	PHE	2.4
1	G	16	GLU	2.4
1	E	35	LEU	2.3
1	C	308	MET	2.3
1	H	217	PRO	2.3
1	H	255	SER	2.3
1	A	64	HIS	2.3
1	A	335	ASP	2.3
1	E	48	PHE	2.3
1	F	188	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	16	GLU	2.3
1	F	117	GLU	2.3
1	G	233	ALA	2.3
1	E	301	THR	2.3
1	D	330	ARG	2.3
1	C	242	SER	2.3
1	H	40	GLY	2.3
1	C	331	LEU	2.3
1	H	174	ASP	2.3
1	A	188	LYS	2.3
1	E	326	LYS	2.3
1	H	219	ALA	2.3
1	G	336	ARG	2.3
1	A	175	SER	2.3
1	G	230	SER	2.3
1	H	254	LEU	2.3
1	G	308	MET	2.3
1	H	304	LYS	2.3
1	E	260	PRO	2.3
1	H	228	ALA	2.2
1	A	257	GLY	2.2
1	A	323	GLN	2.2
1	A	321	LYS	2.2
1	F	3	SER	2.2
1	F	62	LEU	2.2
1	H	310	ILE	2.2
1	A	174	ASP	2.2
1	G	323	GLN	2.2
1	H	333	GLN	2.2
1	D	303	LEU	2.2
1	H	227	SER	2.2
1	H	79	ALA	2.2
1	E	9	GLY	2.2
1	H	284	ILE	2.2
1	H	268	SER	2.2
1	F	319	ARG	2.2
1	C	329	PHE	2.2
1	E	30	PRO	2.2
1	B	36	ALA	2.2
1	H	218	ALA	2.2
1	H	280	ALA	2.2
1	B	221	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	260	PRO	2.2
1	G	263	PHE	2.2
1	G	334	VAL	2.1
1	H	193	VAL	2.1
1	G	219	ALA	2.1
1	H	66	ALA	2.1
1	F	257	GLY	2.1
1	H	35	LEU	2.1
1	F	185	SER	2.1
1	F	246	ASP	2.1
1	B	329	PHE	2.1
1	E	292	HIS	2.1
1	C	63	ALA	2.1
1	F	63	ALA	2.1
1	H	192	LEU	2.1
1	H	303	LEU	2.1
1	B	335	ASP	2.1
1	F	227	SER	2.1
1	H	211	LYS	2.1
1	A	329	PHE	2.1
1	F	64	HIS	2.1
1	G	333	GLN	2.1
1	H	127	VAL	2.1
1	H	129	VAL	2.1
1	B	286	LEU	2.1
1	E	31	LEU	2.1
1	C	282	ARG	2.1
1	B	41	ILE	2.1
1	D	284	ILE	2.1
1	G	41	ILE	2.1
1	F	269	TYR	2.1
1	H	269	TYR	2.1
1	G	227	SER	2.1
1	E	49	ALA	2.1
1	A	319	ARG	2.1
1	F	10	LEU	2.1
1	E	18	GLY	2.1
1	H	134	ARG	2.1
1	D	187	ASP	2.1
1	G	313	ASP	2.1
1	H	205	TYR	2.1
1	A	34	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	218	ALA	2.0
1	B	288	ALA	2.0
1	H	142	LEU	2.0
1	E	188	LYS	2.0
1	B	224	MET	2.0
1	A	189	ARG	2.0
1	A	330	ARG	2.0
1	B	330	ARG	2.0
1	C	334	VAL	2.0
1	F	326	LYS	2.0
1	E	284	ILE	2.0
1	A	226	ASP	2.0
1	E	44	ASP	2.0
1	G	42	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.