



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:36 AM UTC

PDB ID : 4J25 / pdb_00004j25
Title : Crystal structure of a Pseudomonas putida prolyl-4-hydroxylase (P4H)
Authors : Scotti, J.S.; McDonough, M.A.; Schofield, C.J.
Deposited on : 2013-02-04
Resolution : 1.97 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:

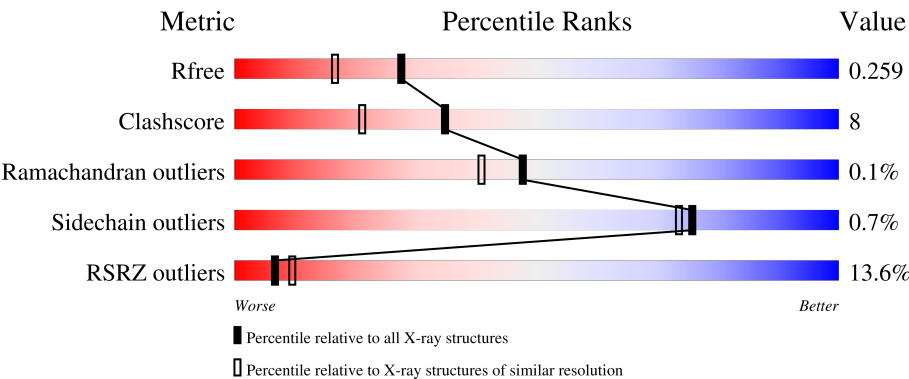
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 1.97 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	229	2% 68%10%21%
1	B	229	% 70%7%23%
1	C	229	3% 69%9%22%
1	D	229	2% 69%10%21%
1	E	229	3% 75%5%20%

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Mol	Chain	Length	Quality of chain
1	F	229	
1	G	229	
1	H	229	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11849 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 Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	1	0
			1432	906	263	256	7			
1	B	177	Total	C	N	O	S	0	0	0
			1377	873	251	245	8			
1	C	179	Total	C	N	O	S	0	0	0
			1377	872	250	247	8			
1	D	181	Total	C	N	O	S	0	0	0
			1415	893	260	255	7			
1	E	184	Total	C	N	O	S	0	0	0
			1417	899	259	251	8			
1	F	187	Total	C	N	O	S	0	0	0
			1399	892	254	246	7			
1	G	184	Total	C	N	O	S	0	0	0
			1378	878	251	241	8			
1	H	186	Total	C	N	O	S	0	0	0
			1403	891	257	247	8			

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP Q88CM1
A	-20	GLY	-	expression tag	UNP Q88CM1
A	-19	SER	-	expression tag	UNP Q88CM1
A	-18	SER	-	expression tag	UNP Q88CM1
A	-17	HIS	-	expression tag	UNP Q88CM1
A	-16	HIS	-	expression tag	UNP Q88CM1
A	-15	HIS	-	expression tag	UNP Q88CM1
A	-14	HIS	-	expression tag	UNP Q88CM1
A	-13	HIS	-	expression tag	UNP Q88CM1
A	-12	HIS	-	expression tag	UNP Q88CM1
A	-11	SER	-	expression tag	UNP Q88CM1
A	-10	SER	-	expression tag	UNP Q88CM1
A	-9	GLY	-	expression tag	UNP Q88CM1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	LEU	-	expression tag	UNP Q88CM1
A	-7	VAL	-	expression tag	UNP Q88CM1
A	-6	PRO	-	expression tag	UNP Q88CM1
A	-5	ARG	-	expression tag	UNP Q88CM1
A	-4	GLY	-	expression tag	UNP Q88CM1
A	-3	SER	-	expression tag	UNP Q88CM1
A	-2	HIS	-	expression tag	UNP Q88CM1
A	-1	MET	-	expression tag	UNP Q88CM1
A	0	ALA	-	expression tag	UNP Q88CM1
A	1	SER	-	expression tag	UNP Q88CM1
B	-21	MET	-	expression tag	UNP Q88CM1
B	-20	GLY	-	expression tag	UNP Q88CM1
B	-19	SER	-	expression tag	UNP Q88CM1
B	-18	SER	-	expression tag	UNP Q88CM1
B	-17	HIS	-	expression tag	UNP Q88CM1
B	-16	HIS	-	expression tag	UNP Q88CM1
B	-15	HIS	-	expression tag	UNP Q88CM1
B	-14	HIS	-	expression tag	UNP Q88CM1
B	-13	HIS	-	expression tag	UNP Q88CM1
B	-12	HIS	-	expression tag	UNP Q88CM1
B	-11	SER	-	expression tag	UNP Q88CM1
B	-10	SER	-	expression tag	UNP Q88CM1
B	-9	GLY	-	expression tag	UNP Q88CM1
B	-8	LEU	-	expression tag	UNP Q88CM1
B	-7	VAL	-	expression tag	UNP Q88CM1
B	-6	PRO	-	expression tag	UNP Q88CM1
B	-5	ARG	-	expression tag	UNP Q88CM1
B	-4	GLY	-	expression tag	UNP Q88CM1
B	-3	SER	-	expression tag	UNP Q88CM1
B	-2	HIS	-	expression tag	UNP Q88CM1
B	-1	MET	-	expression tag	UNP Q88CM1
B	0	ALA	-	expression tag	UNP Q88CM1
B	1	SER	-	expression tag	UNP Q88CM1
C	-21	MET	-	expression tag	UNP Q88CM1
C	-20	GLY	-	expression tag	UNP Q88CM1
C	-19	SER	-	expression tag	UNP Q88CM1
C	-18	SER	-	expression tag	UNP Q88CM1
C	-17	HIS	-	expression tag	UNP Q88CM1
C	-16	HIS	-	expression tag	UNP Q88CM1
C	-15	HIS	-	expression tag	UNP Q88CM1
C	-14	HIS	-	expression tag	UNP Q88CM1
C	-13	HIS	-	expression tag	UNP Q88CM1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	HIS	-	expression tag	UNP Q88CM1
C	-11	SER	-	expression tag	UNP Q88CM1
C	-10	SER	-	expression tag	UNP Q88CM1
C	-9	GLY	-	expression tag	UNP Q88CM1
C	-8	LEU	-	expression tag	UNP Q88CM1
C	-7	VAL	-	expression tag	UNP Q88CM1
C	-6	PRO	-	expression tag	UNP Q88CM1
C	-5	ARG	-	expression tag	UNP Q88CM1
C	-4	GLY	-	expression tag	UNP Q88CM1
C	-3	SER	-	expression tag	UNP Q88CM1
C	-2	HIS	-	expression tag	UNP Q88CM1
C	-1	MET	-	expression tag	UNP Q88CM1
C	0	ALA	-	expression tag	UNP Q88CM1
C	1	SER	-	expression tag	UNP Q88CM1
D	-21	MET	-	expression tag	UNP Q88CM1
D	-20	GLY	-	expression tag	UNP Q88CM1
D	-19	SER	-	expression tag	UNP Q88CM1
D	-18	SER	-	expression tag	UNP Q88CM1
D	-17	HIS	-	expression tag	UNP Q88CM1
D	-16	HIS	-	expression tag	UNP Q88CM1
D	-15	HIS	-	expression tag	UNP Q88CM1
D	-14	HIS	-	expression tag	UNP Q88CM1
D	-13	HIS	-	expression tag	UNP Q88CM1
D	-12	HIS	-	expression tag	UNP Q88CM1
D	-11	SER	-	expression tag	UNP Q88CM1
D	-10	SER	-	expression tag	UNP Q88CM1
D	-9	GLY	-	expression tag	UNP Q88CM1
D	-8	LEU	-	expression tag	UNP Q88CM1
D	-7	VAL	-	expression tag	UNP Q88CM1
D	-6	PRO	-	expression tag	UNP Q88CM1
D	-5	ARG	-	expression tag	UNP Q88CM1
D	-4	GLY	-	expression tag	UNP Q88CM1
D	-3	SER	-	expression tag	UNP Q88CM1
D	-2	HIS	-	expression tag	UNP Q88CM1
D	-1	MET	-	expression tag	UNP Q88CM1
D	0	ALA	-	expression tag	UNP Q88CM1
D	1	SER	-	expression tag	UNP Q88CM1
E	-21	MET	-	expression tag	UNP Q88CM1
E	-20	GLY	-	expression tag	UNP Q88CM1
E	-19	SER	-	expression tag	UNP Q88CM1
E	-18	SER	-	expression tag	UNP Q88CM1
E	-17	HIS	-	expression tag	UNP Q88CM1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-16	HIS	-	expression tag	UNP Q88CM1
E	-15	HIS	-	expression tag	UNP Q88CM1
E	-14	HIS	-	expression tag	UNP Q88CM1
E	-13	HIS	-	expression tag	UNP Q88CM1
E	-12	HIS	-	expression tag	UNP Q88CM1
E	-11	SER	-	expression tag	UNP Q88CM1
E	-10	SER	-	expression tag	UNP Q88CM1
E	-9	GLY	-	expression tag	UNP Q88CM1
E	-8	LEU	-	expression tag	UNP Q88CM1
E	-7	VAL	-	expression tag	UNP Q88CM1
E	-6	PRO	-	expression tag	UNP Q88CM1
E	-5	ARG	-	expression tag	UNP Q88CM1
E	-4	GLY	-	expression tag	UNP Q88CM1
E	-3	SER	-	expression tag	UNP Q88CM1
E	-2	HIS	-	expression tag	UNP Q88CM1
E	-1	MET	-	expression tag	UNP Q88CM1
E	0	ALA	-	expression tag	UNP Q88CM1
E	1	SER	-	expression tag	UNP Q88CM1
F	-21	MET	-	expression tag	UNP Q88CM1
F	-20	GLY	-	expression tag	UNP Q88CM1
F	-19	SER	-	expression tag	UNP Q88CM1
F	-18	SER	-	expression tag	UNP Q88CM1
F	-17	HIS	-	expression tag	UNP Q88CM1
F	-16	HIS	-	expression tag	UNP Q88CM1
F	-15	HIS	-	expression tag	UNP Q88CM1
F	-14	HIS	-	expression tag	UNP Q88CM1
F	-13	HIS	-	expression tag	UNP Q88CM1
F	-12	HIS	-	expression tag	UNP Q88CM1
F	-11	SER	-	expression tag	UNP Q88CM1
F	-10	SER	-	expression tag	UNP Q88CM1
F	-9	GLY	-	expression tag	UNP Q88CM1
F	-8	LEU	-	expression tag	UNP Q88CM1
F	-7	VAL	-	expression tag	UNP Q88CM1
F	-6	PRO	-	expression tag	UNP Q88CM1
F	-5	ARG	-	expression tag	UNP Q88CM1
F	-4	GLY	-	expression tag	UNP Q88CM1
F	-3	SER	-	expression tag	UNP Q88CM1
F	-2	HIS	-	expression tag	UNP Q88CM1
F	-1	MET	-	expression tag	UNP Q88CM1
F	0	ALA	-	expression tag	UNP Q88CM1
F	1	SER	-	expression tag	UNP Q88CM1
G	-21	MET	-	expression tag	UNP Q88CM1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-20	GLY	-	expression tag	UNP Q88CM1
G	-19	SER	-	expression tag	UNP Q88CM1
G	-18	SER	-	expression tag	UNP Q88CM1
G	-17	HIS	-	expression tag	UNP Q88CM1
G	-16	HIS	-	expression tag	UNP Q88CM1
G	-15	HIS	-	expression tag	UNP Q88CM1
G	-14	HIS	-	expression tag	UNP Q88CM1
G	-13	HIS	-	expression tag	UNP Q88CM1
G	-12	HIS	-	expression tag	UNP Q88CM1
G	-11	SER	-	expression tag	UNP Q88CM1
G	-10	SER	-	expression tag	UNP Q88CM1
G	-9	GLY	-	expression tag	UNP Q88CM1
G	-8	LEU	-	expression tag	UNP Q88CM1
G	-7	VAL	-	expression tag	UNP Q88CM1
G	-6	PRO	-	expression tag	UNP Q88CM1
G	-5	ARG	-	expression tag	UNP Q88CM1
G	-4	GLY	-	expression tag	UNP Q88CM1
G	-3	SER	-	expression tag	UNP Q88CM1
G	-2	HIS	-	expression tag	UNP Q88CM1
G	-1	MET	-	expression tag	UNP Q88CM1
G	0	ALA	-	expression tag	UNP Q88CM1
G	1	SER	-	expression tag	UNP Q88CM1
H	-21	MET	-	expression tag	UNP Q88CM1
H	-20	GLY	-	expression tag	UNP Q88CM1
H	-19	SER	-	expression tag	UNP Q88CM1
H	-18	SER	-	expression tag	UNP Q88CM1
H	-17	HIS	-	expression tag	UNP Q88CM1
H	-16	HIS	-	expression tag	UNP Q88CM1
H	-15	HIS	-	expression tag	UNP Q88CM1
H	-14	HIS	-	expression tag	UNP Q88CM1
H	-13	HIS	-	expression tag	UNP Q88CM1
H	-12	HIS	-	expression tag	UNP Q88CM1
H	-11	SER	-	expression tag	UNP Q88CM1
H	-10	SER	-	expression tag	UNP Q88CM1
H	-9	GLY	-	expression tag	UNP Q88CM1
H	-8	LEU	-	expression tag	UNP Q88CM1
H	-7	VAL	-	expression tag	UNP Q88CM1
H	-6	PRO	-	expression tag	UNP Q88CM1
H	-5	ARG	-	expression tag	UNP Q88CM1
H	-4	GLY	-	expression tag	UNP Q88CM1
H	-3	SER	-	expression tag	UNP Q88CM1
H	-2	HIS	-	expression tag	UNP Q88CM1

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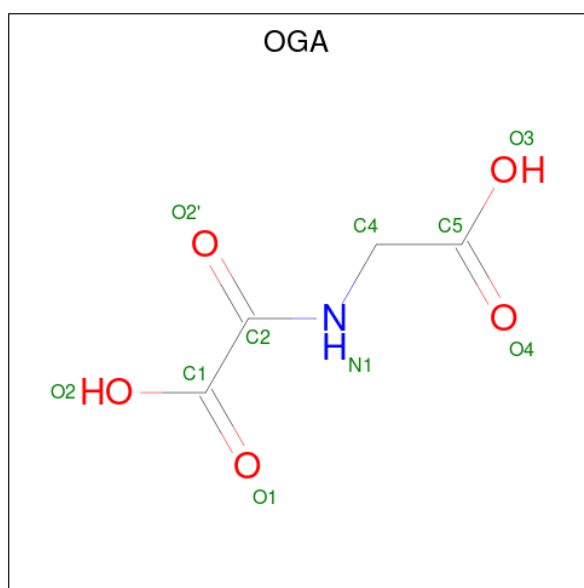
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Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	MET	-	expression tag	UNP Q88CM1
H	0	ALA	-	expression tag	UNP Q88CM1
H	1	SER	-	expression tag	UNP Q88CM1

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		
2	E	1	Total	Mn	0	0
			1	1		
2	F	1	Total	Mn	0	0
			1	1		
2	G	1	Total	Mn	0	0
			1	1		
2	H	1	Total	Mn	0	0
			1	1		

- Molecule 3 is N-OXALYLGLYCINE (CCD ID: OGA) (formula: C₄H₅NO₅).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 10 4 1 5	0	0
3	B	1	Total C N O 10 4 1 5	0	0
3	C	1	Total C N O 10 4 1 5	0	0
3	D	1	Total C N O 10 4 1 5	0	0
3	E	1	Total C N O 10 4 1 5	0	0
3	F	1	Total C N O 10 4 1 5	0	0
3	G	1	Total C N O 10 4 1 5	0	0
3	H	1	Total C N O 10 4 1 5	0	0

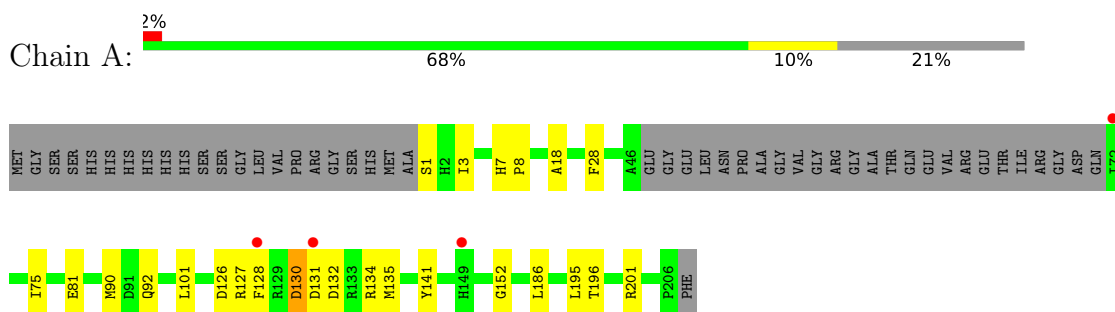
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	93	Total O 93 93	0	0
4	B	100	Total O 100 100	0	0
4	C	88	Total O 88 88	0	0
4	D	89	Total O 89 89	0	0
4	E	51	Total O 51 51	0	0
4	F	51	Total O 51 51	0	0
4	G	39	Total O 39 39	0	0
4	H	52	Total O 52 52	0	0

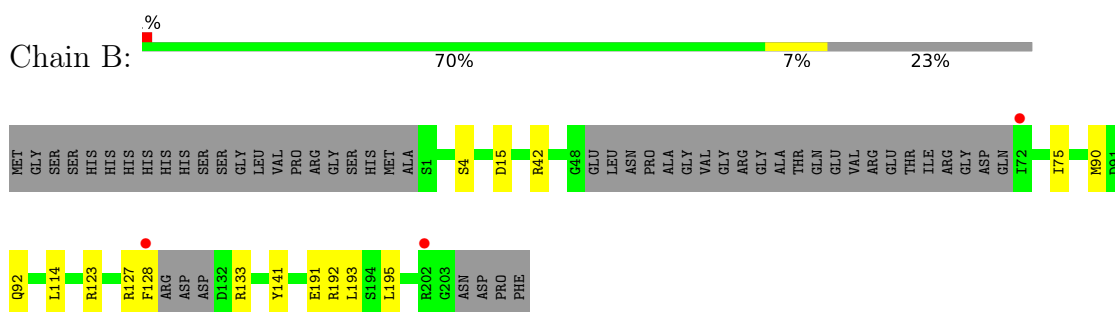
3 Residue-property plots [i](#)

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.

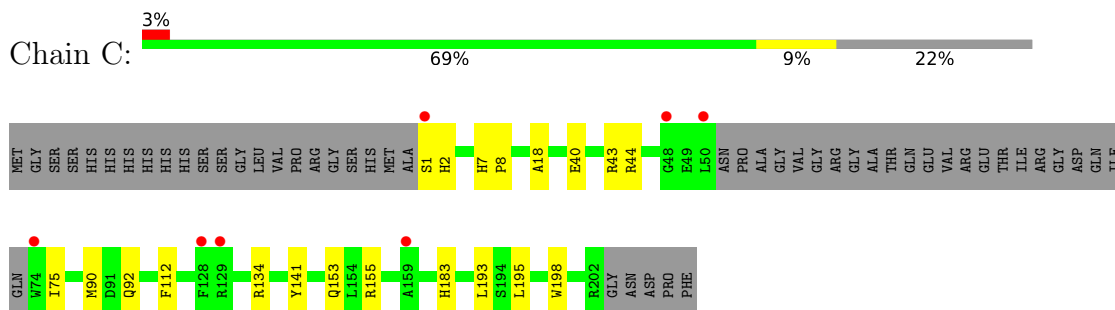
- Molecule 1: Putative uncharacterized protein



- Molecule 1: Putative uncharacterized protein

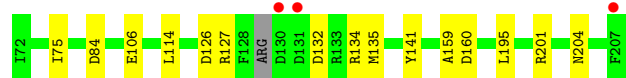


- Molecule 1: Putative uncharacterized protein

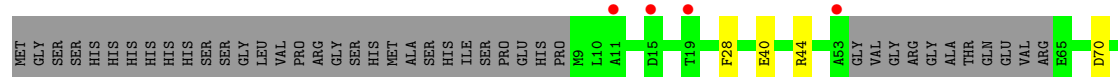
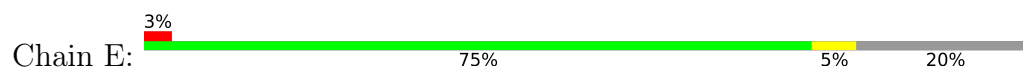


- Molecule 1: Putative uncharacterized protein

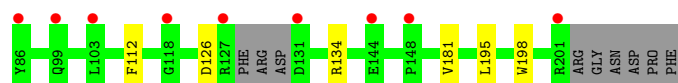
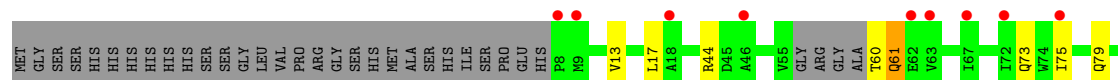
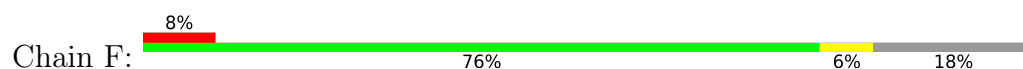




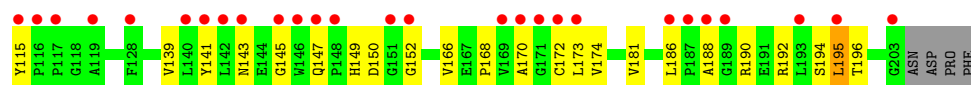
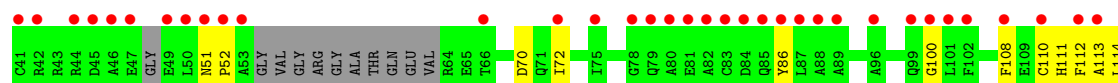
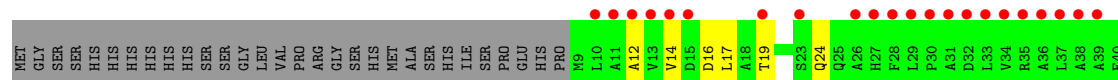
- Molecule 1: Putative uncharacterized protein



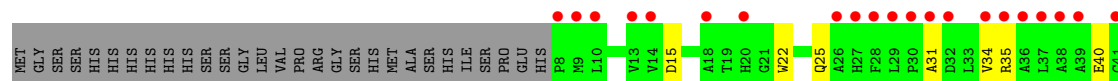
- Molecule 1: Putative uncharacterized protein

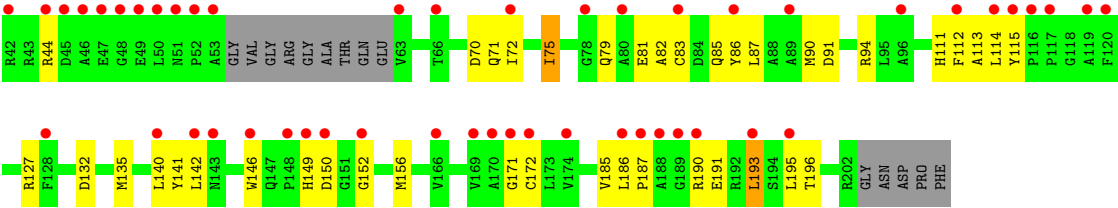


- Molecule 1: Putative uncharacterized protein



- Molecule 1: Putative uncharacterized protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	45.33Å 62.16Å 132.83Å 91.84° 94.70° 90.08°	Depositor
Resolution (Å)	62.13 – 1.97 62.13 – 1.97	Depositor EDS
% Data completeness (in resolution range)	94.7 (62.13-1.97) 88.4 (62.13-1.97)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 1.97Å)	Xtriage
Refinement program	PHENIX 1.8.1 _1168	Depositor
R, R_{free}	0.212 , 0.257 0.217 , 0.259	Depositor DCC
R_{free} test set	2002 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.056 for -h,k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11849	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.28% 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: OGA, MN

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	0.53	0/1474	0.73	0/2004
1	B	0.55	0/1413	0.71	0/1919
1	C	0.55	0/1412	0.72	0/1919
1	D	0.52	0/1451	0.73	0/1970
1	E	0.44	0/1452	0.70	0/1973
1	F	0.45	0/1433	0.70	1/1952 (0.1%)
1	G	0.46	0/1411	0.79	1/1918 (0.1%)
1	H	0.48	0/1438	0.78	0/1957
All	All	0.50	0/11484	0.73	2/15612 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	181	VAL	N-CA-C	6.00	114.09	108.15
1	G	181	VAL	N-CA-C	5.67	113.76	108.15

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	1432	0	1360	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1377	0	1304	13	0
1	C	1377	0	1296	18	0
1	D	1415	0	1336	14	0
1	E	1417	0	1337	10	0
1	F	1399	0	1306	9	0
1	G	1378	0	1270	33	0
1	H	1403	0	1306	45	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	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	1	0	0	0	0
3	A	10	0	3	2	0
3	B	10	0	3	2	0
3	C	10	0	3	2	0
3	D	10	0	3	2	0
3	E	10	0	3	1	0
3	F	10	0	3	0	0
3	G	10	0	3	1	0
3	H	10	0	3	1	0
4	A	93	0	0	3	0
4	B	100	0	0	6	0
4	C	88	0	0	4	0
4	D	89	0	0	4	0
4	E	51	0	0	2	0
4	F	51	0	0	1	0
4	G	39	0	0	2	0
4	H	52	0	0	6	0
All	All	11849	0	10539	164	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 8.

All (164) 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:44:ARG:NH2	1:H:83:CYS:SG	2.52	0.82
1:G:111:HIS:CE1	1:G:196:THR:HG23	2.15	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:402:OGA:O3	4:D:580:HOH:O	1.96	0.81
1:H:127:ARG:NH1	1:H:135:MET:SD	2.54	0.81
1:D:135:MET:SD	4:D:568:HOH:O	2.38	0.81
1:B:141:TYR:OH	3:B:402:OGA:O4	2.00	0.79
1:G:172:CYS:SG	4:G:506:HOH:O	2.41	0.76
3:A:402:OGA:O4	4:A:579:HOH:O	2.03	0.75
1:F:126:ASP:O	1:F:134:ARG:NH2	2.22	0.73
1:F:79:GLN:NE2	4:F:515:HOH:O	2.18	0.71
1:D:126:ASP:O	1:D:134:ARG:NH2	2.24	0.71
1:B:133:ARG:NH2	4:B:595:HOH:O	2.23	0.70
1:F:75:ILE:CD1	1:F:195:LEU:HD11	2.22	0.70
1:C:44:ARG:NH2	4:C:554:HOH:O	2.23	0.70
1:H:141:TYR:O	4:H:529:HOH:O	2.09	0.69
1:H:15:ASP:N	4:H:538:HOH:O	2.25	0.68
1:H:152:GLY:HA2	1:H:186:LEU:O	1.93	0.68
1:B:15:ASP:OD2	4:B:540:HOH:O	2.12	0.67
3:B:402:OGA:O3	4:B:561:HOH:O	2.12	0.66
1:G:147:GLN:CB	1:G:150:ASP:OD2	2.44	0.66
1:D:106:GLU:OE2	4:D:529:HOH:O	2.14	0.66
1:H:185:VAL:O	4:H:506:HOH:O	2.13	0.65
1:F:75:ILE:HD11	1:F:195:LEU:HD11	1.76	0.65
1:H:142:LEU:HB2	1:H:193:LEU:CD1	2.27	0.65
1:C:153:GLN:CD	4:C:519:HOH:O	2.41	0.64
3:E:402:OGA:O4	4:E:524:HOH:O	2.15	0.64
1:H:86:TYR:CD2	1:H:195:LEU:HD21	2.34	0.63
1:H:91:ASP:OD1	1:H:94:ARG:NH1	2.32	0.62
1:A:196[B]:THR:HG23	4:A:512:HOH:O	2.00	0.62
1:H:40:GLU:O	1:H:44:ARG:HG2	2.00	0.61
1:G:141:TYR:OH	3:G:402:OGA:O4	2.17	0.60
1:A:127:ARG:HG3	1:A:132:ASP:HB3	1.82	0.60
1:H:141:TYR:OH	3:H:402:OGA:O4	2.16	0.60
1:H:91:ASP:OD1	1:H:94:ARG:NH2	2.37	0.58
1:C:75:ILE:HD12	1:C:195:LEU:HD11	1.84	0.58
1:A:3:ILE:HD13	1:C:18:ALA:HA	1.85	0.57
1:H:44:ARG:NH1	1:H:79:GLN:OE1	2.37	0.57
1:G:16:ASP:O	1:G:19:THR:N	2.37	0.57
1:G:70:ASP:HB3	1:G:115:TYR:CE1	2.40	0.56
1:B:4:SER:OG	1:B:92:GLN:NE2	2.39	0.56
1:H:114:LEU:HD12	1:H:193:LEU:HB3	1.86	0.56
1:D:141:TYR:OH	3:D:402:OGA:O4	2.22	0.56
1:H:146:TRP:CE3	1:H:190:ARG:NH2	2.74	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:ARG:HG3	1:D:132:ASP:HB3	1.89	0.55
1:G:172:CYS:HB3	4:G:506:HOH:O	2.06	0.55
1:G:72:ILE:HB	1:G:111:HIS:HD2	1.70	0.54
1:H:31:ALA:O	1:H:35:ARG:HG2	2.08	0.54
1:H:70:ASP:HB3	1:H:115:TYR:CE1	2.42	0.54
1:G:24:GLN:O	1:G:24:GLN:HG3	2.09	0.53
1:C:141:TYR:OH	3:C:402:OGA:O3	2.17	0.53
1:A:131:ASP:O	1:A:132:ASP:C	2.50	0.53
1:G:12:ALA:O	1:G:16:ASP:N	2.40	0.53
1:H:171:GLY:N	4:H:529:HOH:O	2.39	0.53
1:A:7:HIS:HE1	1:A:92:GLN:OE1	1.92	0.53
1:A:141:TYR:OH	3:A:402:OGA:O3	2.25	0.53
1:G:115:TYR:HB2	1:G:192:ARG:CG	2.39	0.53
1:G:139:VAL:O	1:G:139:VAL:HG13	2.08	0.53
1:A:196[B]:THR:CG2	4:A:512:HOH:O	2.55	0.52
1:G:70:ASP:HB3	1:G:115:TYR:CZ	2.45	0.52
1:G:72:ILE:HB	1:G:111:HIS:CD2	2.45	0.52
1:E:114:LEU:C	1:E:114:LEU:HD23	2.34	0.52
1:F:44:ARG:HD3	1:F:73:GLN:OE1	2.10	0.52
1:G:72:ILE:CB	1:G:111:HIS:HD2	2.22	0.52
1:B:90:MET:HA	1:B:90:MET:HE2	1.92	0.51
1:H:127:ARG:HG3	1:H:132:ASP:HB3	1.93	0.51
1:G:51:ASN:HB3	1:G:52:PRO:HD2	1.92	0.51
1:H:111:HIS:CE1	1:H:196:THR:CG2	2.94	0.50
1:F:134:ARG:HD2	1:F:198:TRP:CG	2.46	0.50
1:B:92:GLN:NE2	4:B:579:HOH:O	2.42	0.50
1:E:75:ILE:HD12	1:E:195:LEU:HD21	1.94	0.50
1:H:40:GLU:CB	1:H:82:ALA:HB3	2.41	0.50
1:B:123:ARG:NH2	4:B:589:HOH:O	2.43	0.49
1:F:112:PHE:CD1	1:F:195:LEU:HD13	2.48	0.49
1:G:14:VAL:HG11	1:G:100:GLY:HA3	1.94	0.49
1:H:34:VAL:HG11	1:H:171:GLY:HA2	1.95	0.49
1:E:28:PHE:CE2	1:E:90:MET:CE	2.96	0.49
1:G:113:ALA:HB3	1:G:194:SER:OG	2.13	0.49
1:H:75:ILE:HD11	1:H:87:LEU:HD21	1.95	0.49
1:C:7:HIS:HE1	1:C:92:GLN:OE1	1.96	0.48
1:B:193:LEU:HD12	1:B:193:LEU:N	2.29	0.48
1:H:186:LEU:O	1:H:187:PRO:C	2.57	0.48
1:F:60:THR:O	1:F:61:GLN:CB	2.62	0.48
1:C:40:GLU:OE2	1:C:44:ARG:NH1	2.46	0.47
1:C:90:MET:HA	1:C:90:MET:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:SER:HB2	1:A:81:GLU:OE1	2.15	0.47
1:C:40:GLU:OE2	1:C:43:ARG:NH2	2.46	0.47
1:D:44:ARG:O	1:D:45:ASP:CB	2.63	0.47
1:A:7:HIS:HD2	1:A:8:PRO:O	1.96	0.47
1:D:114:LEU:C	1:D:114:LEU:HD23	2.39	0.47
1:H:112:PHE:CE1	1:H:195:LEU:HD13	2.49	0.47
1:C:7:HIS:HD2	1:C:8:PRO:O	1.97	0.47
3:C:402:OGA:O4	4:C:575:HOH:O	2.20	0.47
1:E:40:GLU:O	1:E:44:ARG:HG3	2.14	0.47
1:G:24:GLN:HA	1:G:173:LEU:O	2.14	0.47
1:D:7:HIS:HD2	1:D:8:PRO:O	1.98	0.46
1:A:18:ALA:HB2	1:A:101:LEU:HD21	1.97	0.46
1:C:1:SER:OG	1:C:2:HIS:N	2.45	0.46
1:G:16:ASP:O	1:G:17:LEU:C	2.59	0.46
1:E:152:GLY:HA2	1:E:186:LEU:O	2.15	0.46
1:B:42:ARG:NH2	1:B:191:GLU:OE2	2.47	0.46
1:G:114:LEU:C	1:G:114:LEU:HD23	2.40	0.46
1:B:75:ILE:HD12	1:B:195:LEU:HD11	1.97	0.46
1:H:72:ILE:HA	1:H:112:PHE:O	2.15	0.46
1:E:86:TYR:CE1	1:E:90:MET:HE3	2.51	0.45
1:G:112:PHE:CD1	1:G:195:LEU:CD1	2.99	0.45
1:H:150:ASP:OD1	1:H:190:ARG:HD3	2.16	0.45
1:H:172:CYS:N	4:H:529:HOH:O	2.49	0.45
1:E:28:PHE:CE2	1:E:90:MET:HE1	2.52	0.45
1:C:155:ARG:O	1:C:183:HIS:HA	2.16	0.45
1:G:152:GLY:HA2	1:G:186:LEU:O	2.16	0.45
1:A:128:PHE:C	1:A:130:ASP:H	2.25	0.44
1:C:153:GLN:OE1	4:C:519:HOH:O	2.21	0.44
1:G:108:PHE:CE1	1:G:110:CYS:HB3	2.53	0.44
1:C:75:ILE:HD11	1:C:112:PHE:CE2	2.53	0.44
1:B:114:LEU:C	1:B:114:LEU:HD23	2.43	0.44
1:G:141:TYR:CD1	1:G:168:PRO:HB3	2.52	0.44
1:H:114:LEU:HD11	1:H:191:GLU:CG	2.48	0.44
1:B:127:ARG:CG	1:B:128:PHE:H	2.31	0.43
1:G:145:GLY:O	1:G:190:ARG:NH1	2.51	0.43
1:G:70:ASP:OD1	1:G:70:ASP:N	2.51	0.43
1:H:142:LEU:HB2	1:H:193:LEU:HD12	2.00	0.43
1:D:159:ALA:O	1:D:160:ASP:HB2	2.18	0.43
1:D:204:ASN:ND2	4:D:586:HOH:O	2.39	0.43
1:F:13:VAL:O	1:F:17:LEU:HG	2.19	0.43
1:H:86:TYR:CG	1:H:195:LEU:HD21	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:91:ASP:OD1	1:H:94:ARG:CZ	2.67	0.43
1:H:15:ASP:CB	4:H:538:HOH:O	2.67	0.43
1:A:126:ASP:O	1:A:134:ARG:NH2	2.47	0.43
1:D:75:ILE:CD1	1:D:195:LEU:HD11	2.49	0.43
1:G:150:ASP:O	1:G:188:ALA:HA	2.18	0.43
1:A:135:MET:HG3	1:A:201:ARG:HG3	2.00	0.42
1:A:152:GLY:HA2	1:A:186:LEU:O	2.19	0.42
1:G:112:PHE:CE1	1:G:195:LEU:HD11	2.55	0.42
1:G:115:TYR:HB2	1:G:192:ARG:HG2	2.00	0.42
1:A:28:PHE:CE2	1:A:90:MET:CE	3.03	0.42
1:D:135:MET:HG3	1:D:201:ARG:HG3	2.01	0.42
1:E:44:ARG:HD3	1:E:73:GLN:OE1	2.20	0.42
1:H:71:GLN:O	1:H:113:ALA:HA	2.20	0.42
1:E:70:ASP:OD1	1:E:70:ASP:N	2.53	0.42
1:G:166:VAL:HG11	1:G:174:VAL:CG2	2.50	0.42
1:E:167:GLU:HG2	4:E:526:HOH:O	2.20	0.42
1:D:16:ASP:CB	1:D:23:SER:HB2	2.50	0.41
1:H:75:ILE:CD1	1:H:87:LEU:HD11	2.50	0.41
1:C:134:ARG:HD2	1:C:198:TRP:CG	2.55	0.41
1:H:81:GLU:O	1:H:85:GLN:CG	2.69	0.41
1:C:193:LEU:HD12	1:C:193:LEU:N	2.36	0.41
1:B:192:ARG:HD2	4:B:597:HOH:O	2.21	0.41
1:D:0:ALA:N	1:D:84:ASP:OD2	2.47	0.41
1:G:143:ASN:C	1:G:170:ALA:HB2	2.46	0.41
1:C:40:GLU:CD	1:C:43:ARG:NH2	2.79	0.41
1:H:25:GLN:O	1:H:172:CYS:HA	2.20	0.41
1:H:86:TYR:CZ	1:H:90:MET:CE	3.04	0.41
1:H:113:ALA:O	1:H:193:LEU:HA	2.21	0.41
1:H:22:TRP:HB2	1:H:156:MET:HE1	2.04	0.40
1:A:7:HIS:CE1	1:A:92:GLN:OE1	2.73	0.40
1:C:40:GLU:CD	1:C:43:ARG:HH21	2.29	0.40
1:H:86:TYR:OH	1:H:90:MET:HE3	2.21	0.40
1:H:140:LEU:HB3	1:H:195:LEU:HB3	2.04	0.40
1:A:75:ILE:CD1	1:A:195:LEU:HD11	2.51	0.40
1:A:127:ARG:CG	1:A:132:ASP:HB3	2.49	0.40
1:G:86:TYR:CE2	1:G:195:LEU:HD23	2.55	0.40
1:H:86:TYR:CE1	1:H:90:MET:HE2	2.56	0.40
1:H:75:ILE:HA	1:H:79:GLN:OE1	2.21	0.40
1:H:111:HIS:CE1	1:H:196:THR:HG23	2.56	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	178/229 (78%)	174 (98%)	4 (2%)	0	100	100
1	B	171/229 (75%)	168 (98%)	3 (2%)	0	100	100
1	C	175/229 (76%)	174 (99%)	1 (1%)	0	100	100
1	D	175/229 (76%)	174 (99%)	1 (1%)	0	100	100
1	E	180/229 (79%)	179 (99%)	1 (1%)	0	100	100
1	F	181/229 (79%)	178 (98%)	2 (1%)	1 (1%)	21	12
1	G	178/229 (78%)	161 (90%)	17 (10%)	0	100	100
1	H	182/229 (80%)	174 (96%)	8 (4%)	0	100	100
All	All	1420/1832 (78%)	1382 (97%)	37 (3%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	61	GLN

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	144/184 (78%)	143 (99%)	1 (1%)	76	73
1	B	136/184 (74%)	136 (100%)	0	100	100
1	C	134/184 (73%)	134 (100%)	0	100	100
1	D	140/184 (76%)	140 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	136/184 (74%)	135 (99%)	1 (1%)	76	73
1	F	130/184 (71%)	130 (100%)	0	100	100
1	G	124/184 (67%)	122 (98%)	2 (2%)	55	50
1	H	130/184 (71%)	127 (98%)	3 (2%)	44	37
All	All	1074/1472 (73%)	1067 (99%)	7 (1%)	76	73

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	ASP
1	E	195	LEU
1	G	149	HIS
1	G	195	LEU
1	H	75	ILE
1	H	149	HIS
1	H	193	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	HIS
1	A	24	GLN
1	A	73	GLN
1	B	7	HIS
1	B	20	HIS
1	B	92	GLN
1	C	7	HIS
1	D	7	HIS
1	D	147	GLN
1	G	51	ASN
1	G	85	GLN
1	G	111	HIS
1	H	25	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](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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	OGA	F	402	2	9,9,9	2.59	2 (22%)	8,11,11	1.66	3 (37%)
3	OGA	C	402	2	9,9,9	2.49	2 (22%)	8,11,11	1.65	2 (25%)
3	OGA	A	402	2	9,9,9	2.69	2 (22%)	8,11,11	1.29	0
3	OGA	E	402	2	9,9,9	2.57	2 (22%)	8,11,11	1.68	3 (37%)
3	OGA	G	402	2	9,9,9	2.46	2 (22%)	8,11,11	1.73	2 (25%)
3	OGA	H	402	2	9,9,9	2.54	2 (22%)	8,11,11	1.55	1 (12%)
3	OGA	B	402	2	9,9,9	2.75	2 (22%)	8,11,11	1.72	3 (37%)
3	OGA	D	402	2	9,9,9	2.58	2 (22%)	8,11,11	2.01	3 (37%)

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	OGA	F	402	2	-	1/8/9/9	-
3	OGA	C	402	2	-	0/8/9/9	-
3	OGA	A	402	2	-	0/8/9/9	-
3	OGA	E	402	2	-	0/8/9/9	-
3	OGA	G	402	2	-	6/8/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OGA	H	402	2	-	1/8/9/9	-
3	OGA	B	402	2	-	2/8/9/9	-
3	OGA	D	402	2	-	0/8/9/9	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	OGA	C2-N1	6.69	1.45	1.33
3	B	402	OGA	C2-N1	6.56	1.44	1.33
3	D	402	OGA	C2-N1	6.54	1.44	1.33
3	C	402	OGA	C2-N1	6.17	1.44	1.33
3	E	402	OGA	C2-N1	6.14	1.44	1.33
3	F	402	OGA	C2-N1	6.09	1.44	1.33
3	G	402	OGA	C2-N1	5.93	1.43	1.33
3	H	402	OGA	C2-N1	5.77	1.43	1.33
3	B	402	OGA	C2-C1	-4.16	1.49	1.54
3	H	402	OGA	C2-C1	-3.87	1.49	1.54
3	F	402	OGA	C2-C1	-3.75	1.49	1.54
3	E	402	OGA	C2-C1	-3.73	1.49	1.54
3	A	402	OGA	C2-C1	-3.45	1.50	1.54
3	C	402	OGA	C2-C1	-3.25	1.50	1.54
3	D	402	OGA	C2-C1	-3.18	1.50	1.54
3	G	402	OGA	C2-C1	-3.05	1.50	1.54

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	OGA	C4-N1-C2	-2.88	116.85	121.29
3	G	402	OGA	O2'-C2-N1	-2.80	118.30	123.35
3	D	402	OGA	O2'-C2-N1	-2.73	118.42	123.35
3	D	402	OGA	O3-C5-C4	2.70	123.07	112.81
3	H	402	OGA	O2'-C2-N1	-2.64	118.59	123.35
3	E	402	OGA	O2'-C2-C1	-2.48	118.10	121.36
3	B	402	OGA	C4-N1-C2	-2.40	117.59	121.29
3	B	402	OGA	O3-C5-C4	2.38	121.85	112.81
3	F	402	OGA	O3-C5-C4	2.37	121.82	112.81
3	C	402	OGA	O2'-C2-N1	-2.33	119.14	123.35
3	B	402	OGA	O2'-C2-C1	-2.32	118.30	121.36
3	G	402	OGA	O3-C5-C4	2.28	121.47	112.81
3	C	402	OGA	O3-C5-O4	-2.25	117.55	123.33
3	F	402	OGA	O2'-C2-N1	-2.21	119.37	123.35
3	E	402	OGA	C4-N1-C2	-2.20	117.90	121.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	402	OGA	O2'-C2-C1	-2.07	118.63	121.36
3	E	402	OGA	O2'-C2-N1	-2.07	119.61	123.35

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	402	OGA	O2-C1-C2-O2'
3	G	402	OGA	O1-C1-C2-O2'
3	G	402	OGA	O2-C1-C2-O2'
3	H	402	OGA	O2-C1-C2-O2'
3	G	402	OGA	O1-C1-C2-N1
3	B	402	OGA	N1-C4-C5-O4
3	G	402	OGA	N1-C4-C5-O4
3	G	402	OGA	C5-C4-N1-C2
3	B	402	OGA	N1-C4-C5-O3
3	G	402	OGA	N1-C4-C5-O3

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	OGA	2	0
3	A	402	OGA	2	0
3	E	402	OGA	1	0
3	G	402	OGA	1	0
3	H	402	OGA	1	0
3	B	402	OGA	2	0
3	D	402	OGA	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

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	181/229 (79%)	0.08	4 (2%) 62 71	11, 23, 43, 62	1 (0%)
1	B	177/229 (77%)	0.07	3 (1%) 69 78	11, 23, 47, 73	0
1	C	179/229 (78%)	0.17	7 (3%) 43 53	13, 24, 53, 80	0
1	D	181/229 (79%)	0.18	5 (2%) 55 65	14, 25, 48, 65	0
1	E	184/229 (80%)	0.54	7 (3%) 44 54	19, 34, 52, 61	0
1	F	187/229 (81%)	0.91	18 (9%) 13 19	26, 39, 54, 76	0
1	G	184/229 (80%)	1.90	84 (45%) 0 0	24, 50, 69, 81	0
1	H	186/229 (81%)	1.61	70 (37%) 1 0	20, 45, 61, 82	0
All	All	1459/1832 (79%)	0.69	198 (13%) 7 9	11, 32, 61, 82	1 (0%)

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	41	CYS	5.6
1	G	101	LEU	5.1
1	G	31	ALA	5.0
1	G	34	VAL	4.5
1	G	47	GLU	4.5
1	D	0	ALA	4.4
1	F	8	PRO	4.4
1	G	146	TRP	4.4
1	H	10	LEU	4.3
1	H	45	ASP	4.3
1	H	50	LEU	4.2
1	G	80	ALA	4.2
1	H	46	ALA	4.2
1	G	38	ALA	4.2
1	G	189	GLY	4.2
1	G	88	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	G	142	LEU	4.1
1	H	148	PRO	4.0
1	D	207	PHE	4.0
1	H	37	LEU	4.0
1	G	119	ALA	4.0
1	H	53	ALA	4.0
1	G	152	GLY	3.9
1	G	39	ALA	3.9
1	C	128	PHE	3.9
1	G	86	TYR	3.8
1	G	87	LEU	3.8
1	G	140	LEU	3.8
1	H	8	PRO	3.8
1	G	169	VAL	3.7
1	G	29	LEU	3.7
1	H	49	GLU	3.7
1	B	128	PHE	3.7
1	H	114	LEU	3.6
1	G	84	ASP	3.6
1	H	9	MET	3.6
1	G	145	GLY	3.6
1	G	13	VAL	3.6
1	H	116	PRO	3.6
1	G	188	ALA	3.5
1	G	53	ALA	3.5
1	H	39	ALA	3.5
1	G	203	GLY	3.5
1	G	32	ASP	3.5
1	H	34	VAL	3.5
1	G	112	PHE	3.5
1	G	100	GLY	3.5
1	G	45	ASP	3.5
1	G	35	ARG	3.5
1	G	26	ALA	3.4
1	G	195	LEU	3.4
1	H	115	TYR	3.4
1	H	149	HIS	3.4
1	E	102	PHE	3.4
1	G	28	PHE	3.4
1	H	63	VAL	3.3
1	H	26	ALA	3.3
1	H	170	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	H	146	TRP	3.3
1	H	117	PRO	3.3
1	G	50	LEU	3.3
1	H	128	PHE	3.3
1	H	44	ARG	3.3
1	G	36	ALA	3.2
1	G	46	ALA	3.2
1	G	41	CYS	3.2
1	H	188	ALA	3.1
1	C	50	LEU	3.1
1	G	83	CYS	3.1
1	G	172	CYS	3.1
1	A	128	PHE	3.1
1	C	129	ARG	3.1
1	H	172	CYS	3.1
1	E	53	ALA	3.1
1	G	11	ALA	3.1
1	G	10	LEU	3.0
1	G	102	PHE	3.0
1	H	36	ALA	3.0
1	G	116	PRO	3.0
1	B	72	ILE	3.0
1	C	74	TRP	3.0
1	H	66	THR	3.0
1	G	30	PRO	3.0
1	H	52	PRO	3.0
1	H	47	GLU	3.0
1	G	37	LEU	2.9
1	H	193	LEU	2.9
1	C	1	SER	2.9
1	H	86	TYR	2.9
1	G	147	GLN	2.9
1	A	131	ASP	2.9
1	H	13	VAL	2.9
1	H	30	PRO	2.9
1	H	31	ALA	2.9
1	F	9	MET	2.9
1	H	35	ARG	2.8
1	G	170	ALA	2.8
1	D	131	ASP	2.8
1	G	19	THR	2.8
1	F	127	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	75	ILE	2.7
1	H	169	VAL	2.7
1	G	82	ALA	2.7
1	G	115	TYR	2.7
1	G	117	PRO	2.7
1	H	80	ALA	2.7
1	G	78	GLY	2.7
1	G	52	PRO	2.7
1	G	148	PRO	2.7
1	G	72	ILE	2.7
1	H	51	ASN	2.7
1	H	27	HIS	2.7
1	E	203	GLY	2.6
1	G	14	VAL	2.6
1	C	159	ALA	2.6
1	G	89	ALA	2.6
1	G	96	ALA	2.6
1	H	38	ALA	2.6
1	H	150	ASP	2.6
1	G	79	GLN	2.6
1	E	103	LEU	2.6
1	G	33	LEU	2.6
1	G	44	ARG	2.6
1	H	119	ALA	2.6
1	H	166	VAL	2.6
1	G	66	THR	2.6
1	G	108	PHE	2.6
1	G	193	LEU	2.6
1	H	29	LEU	2.6
1	F	103	LEU	2.5
1	G	173	LEU	2.5
1	E	11	ALA	2.5
1	G	12	ALA	2.5
1	G	187	PRO	2.5
1	G	51	ASN	2.5
1	G	49	GLU	2.5
1	H	120	PHE	2.5
1	F	99	GLN	2.5
1	G	113	ALA	2.5
1	G	42	ARG	2.4
1	G	85	GLN	2.4
1	G	143	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	48	GLY	2.4
1	H	189	GLY	2.4
1	G	186	LEU	2.4
1	H	18	ALA	2.4
1	H	89	ALA	2.4
1	F	62	GLU	2.4
1	G	81	GLU	2.4
1	H	187	PRO	2.4
1	C	48	GLY	2.4
1	G	151	GLY	2.4
1	G	171	GLY	2.4
1	H	14	VAL	2.4
1	H	152	GLY	2.4
1	E	15	ASP	2.3
1	H	140	LEU	2.3
1	A	72	ILE	2.3
1	F	201	ARG	2.3
1	G	15	ASP	2.3
1	G	128	PHE	2.3
1	H	96	ALA	2.3
1	F	75	ILE	2.3
1	H	190	ARG	2.3
1	H	32	ASP	2.3
1	D	2	HIS	2.3
1	G	110	CYS	2.3
1	H	142	LEU	2.3
1	F	72	ILE	2.2
1	H	20	HIS	2.2
1	G	23	SER	2.2
1	F	18	ALA	2.2
1	H	28	PHE	2.2
1	G	27	HIS	2.2
1	G	99	GLN	2.2
1	H	42	ARG	2.2
1	H	143	ASN	2.2
1	F	63	VAL	2.2
1	A	149	HIS	2.1
1	H	72	ILE	2.1
1	H	171	GLY	2.1
1	F	144	GLU	2.1
1	F	46	ALA	2.1
1	H	112	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	148	PRO	2.1
1	E	19	THR	2.1
1	H	174	VAL	2.1
1	H	83	CYS	2.1
1	H	186	LEU	2.1
1	B	202	ARG	2.1
1	F	67	ILE	2.0
1	F	118	GLY	2.0
1	H	78	GLY	2.0
1	H	195	LEU	2.0
1	D	130	ASP	2.0
1	F	131	ASP	2.0
1	F	86	TYR	2.0
1	G	141	TYR	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
3	OGA	H	402	10/10	0.86	0.10	27,29,32,32	0
3	OGA	G	402	10/10	0.88	0.09	30,31,32,35	0
3	OGA	F	402	10/10	0.91	0.08	28,29,31,32	0
3	OGA	A	402	10/10	0.91	0.08	24,26,27,29	0
3	OGA	C	402	10/10	0.91	0.07	23,26,27,29	0
3	OGA	B	402	10/10	0.92	0.07	24,26,27,27	0
3	OGA	E	402	10/10	0.94	0.07	23,25,27,28	0
3	OGA	D	402	10/10	0.94	0.07	25,28,29,30	0
2	MN	G	401	1/1	0.97	0.04	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	H	401	1/1	0.97	0.04	19,19,19,19	0
2	MN	C	401	1/1	0.98	0.03	20,20,20,20	0
2	MN	F	401	1/1	0.98	0.07	29,29,29,29	0
2	MN	B	401	1/1	0.98	0.03	19,19,19,19	0
2	MN	D	401	1/1	0.99	0.02	17,17,17,17	0
2	MN	A	401	1/1	0.99	0.06	21,21,21,21	0
2	MN	E	401	1/1	1.00	0.01	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.