



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2017 – 09:57 AM EDT

PDB ID : 2OBA  
Title : Pseudomonas aeruginosa 6-pyruvoyl tetrahydrobiopterin synthase  
Authors : McGrath, T.E.; Kisselman, G.; Battaile, K.; Romanov, V.; Wu-Brown, J.; Guthrie, J.; Virag, C.; Mansoury, K.; Edwards, A.M.; Pai, E.F.; Chirgadze, N.Y.  
Deposited on : unknown  
Resolution : 2.33 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

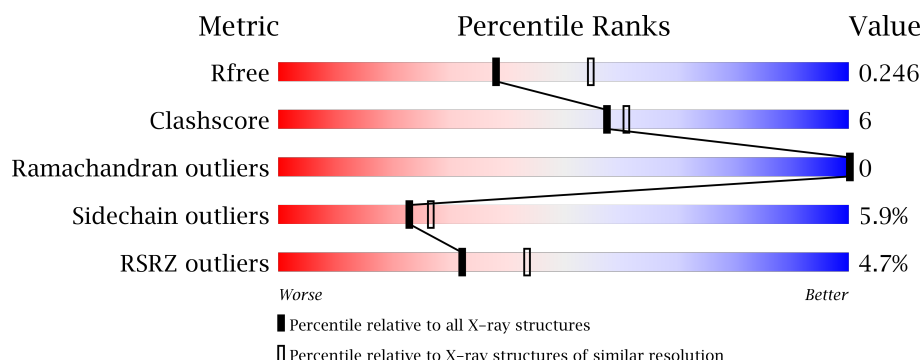
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.33 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))
$R_{free}$	100719	1570 (2.36-2.32)
Clashscore	112137	1673 (2.36-2.32)
Ramachandran outliers	110173	1654 (2.36-2.32)
Sidechain outliers	110143	1655 (2.36-2.32)
RSRZ outliers	101464	1576 (2.36-2.32)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	138	<div> <div>4%</div> <div>72%</div> <div>14%</div> <div>•</div> <div>13%</div> </div>
1	B	138	<div> <div>4%</div> <div>61%</div> <div>25%</div> <div>•</div> <div>12%</div> </div>
1	C	138	<div> <div>2%</div> <div>75%</div> <div>13%</div> <div>•</div> <div>12%</div> </div>
1	D	138	<div> <div>4%</div> <div>76%</div> <div>10%</div> <div>•</div> <div>13%</div> </div>
1	E	138	<div> <div>6%</div> <div>72%</div> <div>14%</div> <div>•</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	138	<div><div></div><div>4%</div><div>70%</div><div>17%</div><div>•</div><div>12%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6228 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 Probable 6-pyruvoyl tetrahydrobiopterin synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	120	Total	C	N	O	S	Se	0	1	0
			994	635	177	177	4	1			
1	B	121	Total	C	N	O	S	Se	0	0	0
			993	632	178	178	4	1			
1	C	121	Total	C	N	O	S	Se	0	0	0
			993	632	178	178	4	1			
1	D	120	Total	C	N	O	S	Se	0	0	0
			989	630	177	177	4	1			
1	E	121	Total	C	N	O	S	Se	0	1	0
			1001	637	181	178	4	1			
1	F	121	Total	C	N	O	S	Se	0	0	0
			993	632	178	178	4	1			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	SEE REMARK 999	UNP Q9I0H2
A	-18	GLY	-	CLONING ARTIFACT	UNP Q9I0H2
A	-17	SER	-	CLONING ARTIFACT	UNP Q9I0H2
A	-16	SER	-	CLONING ARTIFACT	UNP Q9I0H2
A	-15	HIS	-	EXPRESSION TAG	UNP Q9I0H2
A	-14	HIS	-	EXPRESSION TAG	UNP Q9I0H2
A	-13	HIS	-	EXPRESSION TAG	UNP Q9I0H2
A	-12	HIS	-	EXPRESSION TAG	UNP Q9I0H2
A	-11	HIS	-	EXPRESSION TAG	UNP Q9I0H2
A	-10	HIS	-	EXPRESSION TAG	UNP Q9I0H2
A	-9	SER	-	CLONING ARTIFACT	UNP Q9I0H2
A	-8	SER	-	CLONING ARTIFACT	UNP Q9I0H2
A	-7	GLY	-	CLONING ARTIFACT	UNP Q9I0H2
A	-6	LEU	-	CLONING ARTIFACT	UNP Q9I0H2
A	-5	VAL	-	CLONING ARTIFACT	UNP Q9I0H2
A	-4	PRO	-	CLONING ARTIFACT	UNP Q9I0H2
A	-3	ARG	-	CLONING ARTIFACT	UNP Q9I0H2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	CLONING ARTIFACT	UNP Q9I0H2
A	-1	SER	-	CLONING ARTIFACT	UNP Q9I0H2
A	0	HIS	-	CLONING ARTIFACT	UNP Q9I0H2
A	1	MSE	-	CLONING ARTIFACT	UNP Q9I0H2
B	-19	MSE	-	SEE REMARK 999	UNP Q9I0H2
B	-18	GLY	-	CLONING ARTIFACT	UNP Q9I0H2
B	-17	SER	-	CLONING ARTIFACT	UNP Q9I0H2
B	-16	SER	-	CLONING ARTIFACT	UNP Q9I0H2
B	-15	HIS	-	EXPRESSION TAG	UNP Q9I0H2
B	-14	HIS	-	EXPRESSION TAG	UNP Q9I0H2
B	-13	HIS	-	EXPRESSION TAG	UNP Q9I0H2
B	-12	HIS	-	EXPRESSION TAG	UNP Q9I0H2
B	-11	HIS	-	EXPRESSION TAG	UNP Q9I0H2
B	-10	HIS	-	EXPRESSION TAG	UNP Q9I0H2
B	-9	SER	-	CLONING ARTIFACT	UNP Q9I0H2
B	-8	SER	-	CLONING ARTIFACT	UNP Q9I0H2
B	-7	GLY	-	CLONING ARTIFACT	UNP Q9I0H2
B	-6	LEU	-	CLONING ARTIFACT	UNP Q9I0H2
B	-5	VAL	-	CLONING ARTIFACT	UNP Q9I0H2
B	-4	PRO	-	CLONING ARTIFACT	UNP Q9I0H2
B	-3	ARG	-	CLONING ARTIFACT	UNP Q9I0H2
B	-2	GLY	-	CLONING ARTIFACT	UNP Q9I0H2
B	-1	SER	-	CLONING ARTIFACT	UNP Q9I0H2
B	0	HIS	-	CLONING ARTIFACT	UNP Q9I0H2
B	1	MSE	-	CLONING ARTIFACT	UNP Q9I0H2
C	-19	MSE	-	SEE REMARK 999	UNP Q9I0H2
C	-18	GLY	-	CLONING ARTIFACT	UNP Q9I0H2
C	-17	SER	-	CLONING ARTIFACT	UNP Q9I0H2
C	-16	SER	-	CLONING ARTIFACT	UNP Q9I0H2
C	-15	HIS	-	EXPRESSION TAG	UNP Q9I0H2
C	-14	HIS	-	EXPRESSION TAG	UNP Q9I0H2
C	-13	HIS	-	EXPRESSION TAG	UNP Q9I0H2
C	-12	HIS	-	EXPRESSION TAG	UNP Q9I0H2
C	-11	HIS	-	EXPRESSION TAG	UNP Q9I0H2
C	-10	HIS	-	EXPRESSION TAG	UNP Q9I0H2
C	-9	SER	-	CLONING ARTIFACT	UNP Q9I0H2
C	-8	SER	-	CLONING ARTIFACT	UNP Q9I0H2
C	-7	GLY	-	CLONING ARTIFACT	UNP Q9I0H2
C	-6	LEU	-	CLONING ARTIFACT	UNP Q9I0H2
C	-5	VAL	-	CLONING ARTIFACT	UNP Q9I0H2
C	-4	PRO	-	CLONING ARTIFACT	UNP Q9I0H2
C	-3	ARG	-	CLONING ARTIFACT	UNP Q9I0H2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	CLONING ARTIFACT	UNP Q9I0H2
C	-1	SER	-	CLONING ARTIFACT	UNP Q9I0H2
C	0	HIS	-	CLONING ARTIFACT	UNP Q9I0H2
C	1	MSE	-	CLONING ARTIFACT	UNP Q9I0H2
D	-19	MSE	-	SEE REMARK 999	UNP Q9I0H2
D	-18	GLY	-	CLONING ARTIFACT	UNP Q9I0H2
D	-17	SER	-	CLONING ARTIFACT	UNP Q9I0H2
D	-16	SER	-	CLONING ARTIFACT	UNP Q9I0H2
D	-15	HIS	-	EXPRESSION TAG	UNP Q9I0H2
D	-14	HIS	-	EXPRESSION TAG	UNP Q9I0H2
D	-13	HIS	-	EXPRESSION TAG	UNP Q9I0H2
D	-12	HIS	-	EXPRESSION TAG	UNP Q9I0H2
D	-11	HIS	-	EXPRESSION TAG	UNP Q9I0H2
D	-10	HIS	-	EXPRESSION TAG	UNP Q9I0H2
D	-9	SER	-	CLONING ARTIFACT	UNP Q9I0H2
D	-8	SER	-	CLONING ARTIFACT	UNP Q9I0H2
D	-7	GLY	-	CLONING ARTIFACT	UNP Q9I0H2
D	-6	LEU	-	CLONING ARTIFACT	UNP Q9I0H2
D	-5	VAL	-	CLONING ARTIFACT	UNP Q9I0H2
D	-4	PRO	-	CLONING ARTIFACT	UNP Q9I0H2
D	-3	ARG	-	CLONING ARTIFACT	UNP Q9I0H2
D	-2	GLY	-	CLONING ARTIFACT	UNP Q9I0H2
D	-1	SER	-	CLONING ARTIFACT	UNP Q9I0H2
D	0	HIS	-	CLONING ARTIFACT	UNP Q9I0H2
D	1	MSE	-	CLONING ARTIFACT	UNP Q9I0H2
E	-19	MSE	-	SEE REMARK 999	UNP Q9I0H2
E	-18	GLY	-	CLONING ARTIFACT	UNP Q9I0H2
E	-17	SER	-	CLONING ARTIFACT	UNP Q9I0H2
E	-16	SER	-	CLONING ARTIFACT	UNP Q9I0H2
E	-15	HIS	-	EXPRESSION TAG	UNP Q9I0H2
E	-14	HIS	-	EXPRESSION TAG	UNP Q9I0H2
E	-13	HIS	-	EXPRESSION TAG	UNP Q9I0H2
E	-12	HIS	-	EXPRESSION TAG	UNP Q9I0H2
E	-11	HIS	-	EXPRESSION TAG	UNP Q9I0H2
E	-10	HIS	-	EXPRESSION TAG	UNP Q9I0H2
E	-9	SER	-	CLONING ARTIFACT	UNP Q9I0H2
E	-8	SER	-	CLONING ARTIFACT	UNP Q9I0H2
E	-7	GLY	-	CLONING ARTIFACT	UNP Q9I0H2
E	-6	LEU	-	CLONING ARTIFACT	UNP Q9I0H2
E	-5	VAL	-	CLONING ARTIFACT	UNP Q9I0H2
E	-4	PRO	-	CLONING ARTIFACT	UNP Q9I0H2
E	-3	ARG	-	CLONING ARTIFACT	UNP Q9I0H2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	CLONING ARTIFACT	UNP Q9I0H2
E	-1	SER	-	CLONING ARTIFACT	UNP Q9I0H2
E	0	HIS	-	CLONING ARTIFACT	UNP Q9I0H2
E	1	MSE	-	CLONING ARTIFACT	UNP Q9I0H2
F	-19	MSE	-	SEE REMARK 999	UNP Q9I0H2
F	-18	GLY	-	CLONING ARTIFACT	UNP Q9I0H2
F	-17	SER	-	CLONING ARTIFACT	UNP Q9I0H2
F	-16	SER	-	CLONING ARTIFACT	UNP Q9I0H2
F	-15	HIS	-	EXPRESSION TAG	UNP Q9I0H2
F	-14	HIS	-	EXPRESSION TAG	UNP Q9I0H2
F	-13	HIS	-	EXPRESSION TAG	UNP Q9I0H2
F	-12	HIS	-	EXPRESSION TAG	UNP Q9I0H2
F	-11	HIS	-	EXPRESSION TAG	UNP Q9I0H2
F	-10	HIS	-	EXPRESSION TAG	UNP Q9I0H2
F	-9	SER	-	CLONING ARTIFACT	UNP Q9I0H2
F	-8	SER	-	CLONING ARTIFACT	UNP Q9I0H2
F	-7	GLY	-	CLONING ARTIFACT	UNP Q9I0H2
F	-6	LEU	-	CLONING ARTIFACT	UNP Q9I0H2
F	-5	VAL	-	CLONING ARTIFACT	UNP Q9I0H2
F	-4	PRO	-	CLONING ARTIFACT	UNP Q9I0H2
F	-3	ARG	-	CLONING ARTIFACT	UNP Q9I0H2
F	-2	GLY	-	CLONING ARTIFACT	UNP Q9I0H2
F	-1	SER	-	CLONING ARTIFACT	UNP Q9I0H2
F	0	HIS	-	CLONING ARTIFACT	UNP Q9I0H2
F	1	MSE	-	CLONING ARTIFACT	UNP Q9I0H2

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

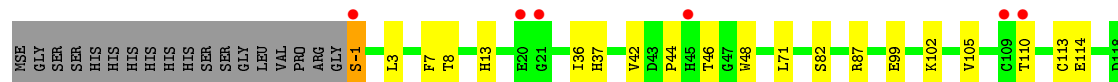
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	63	Total 63	O 63	0	0
3	B	32	Total 32	O 32	0	0
3	C	45	Total 45	O 45	0	0
3	D	52	Total 52	O 52	0	0
3	E	31	Total 31	O 31	0	0
3	F	36	Total 36	O 36	0	0





- Molecule 1: Probable 6-pyruvoyl tetrahydrobiopterin synthase



The diagram illustrates a network of nodes and their connections. The nodes are arranged in a grid-like fashion, with some nodes having red dots above them. The nodes are labeled with codes such as MSE, GLY, SER, HIS, ARG, G-2, S-1, H0, M1, E2, I3, F4, F9, E10, S11, A12, H13, R14, L15, E20, C24, R33, V34, A35, I36, H37, I38, V42, W48, I49, R50, I55, K60, P61, I62, Y63, E64, Q65, L66, L71, S82, E83, W84, L85, C86, R87, Q92, L93, K94, E99, K102, Y103, R104, C109, E114, D118. The connections are represented by lines between the nodes, forming a complex web of relationships.

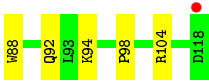
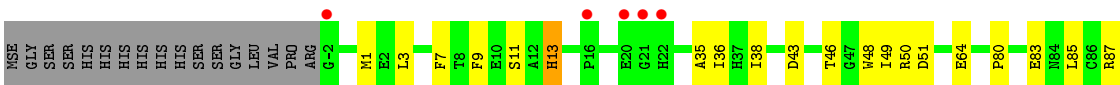
MSE	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	GLY	LEU	VAL	PRO	ARG	G-2	S-1	L3	P-4	K5	H13	R33	H37	I38	W48	I49	R50	D51	E54	I55	L71	O86	L93	K102	C109	T110	S111	G112	D118
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MSE	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	VAL	ARG	PRO	ARG	GLY	S-I	H0	L3	S11	A12	H13	E20	V34	H37	V42	H45	V48	L71	L93	K102	V103	R104	V105	H106	E107	T108	C109	E114	V115	R116	C117	S118
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Category	Item	Value	Color
A	MSE	0.0000	Gray
	GLY	0.0000	Gray
	SER	0.0000	Gray
	SER	0.0000	Gray
	HIS	0.0000	Gray
	HIS	0.0000	Gray
	HIS	0.0000	Gray
	HIS	0.0000	Gray
	HIS	0.0000	Gray
	HIS	0.0000	Gray
B	SER	0.0000	Gray
	SER	0.0000	Gray
	GLY	0.0000	Gray
	VAL	0.0000	Gray
	LEU	0.0000	Gray
	ARG	0.0000	Gray
	ARG	0.0000	Gray
	G-2	0.0000	Red
	S-1	0.0000	Red
	H-0	0.0000	Red
C	F7	0.0000	Yellow
	S11	0.0000	Yellow
	A12	0.0000	Yellow
	H13	0.0000	Yellow
	R14	0.0000	Yellow
	E20	0.0000	Red
	G21	0.0000	Red
	H30	0.0000	Yellow
	V34	0.0000	Yellow
	H37	0.0000	Yellow
D	P44	0.0000	Red
	H45	0.0000	Red
	W48	0.0000	Orange
	K56	0.0000	Yellow
	L71	0.0000	Orange
	S82	0.0000	Yellow
	E83	0.0000	Yellow
	W88	0.0000	Yellow
	Q92	0.0000	Yellow
	K102	0.0000	Yellow
E	V103	0.0000	Yellow
	R104	0.0000	Yellow
	E107	0.0000	Yellow
	T108	0.0000	Green



● Molecule 1: Probable 6-pyruvoyl tetrahydrobiopterin synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.08 Å 87.52 Å 124.67 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.22 – 2.33 42.23 – 2.33	Depositor EDS
% Data completeness (in resolution range)	97.7 (42.22-2.33) 97.7 (42.23-2.33)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.79 (at 2.32 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.186 , 0.256 0.182 , 0.246	Depositor DCC
$R_{free}$ test set	1767 reflections (5.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.8	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 38.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6228	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.37% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.88	2/1028 (0.2%)	0.76	0/1392
1	B	0.68	0/1024	0.75	0/1386
1	C	0.70	1/1024 (0.1%)	0.72	0/1386
1	D	0.81	0/1020	0.77	0/1381
1	E	0.58	0/1035	0.67	0/1400
1	F	0.64	0/1024	0.73	4/1386 (0.3%)
All	All	0.72	3/6155 (0.0%)	0.73	4/8331 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	46	THR	C-O	9.57	1.41	1.23
1	A	44	PRO	C-N	6.03	1.48	1.34
1	C	86	CYS	CB-SG	-5.16	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	50	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	F	51	ASP	CB-CG-OD1	5.26	123.03	118.30
1	F	85	LEU	CA-CB-CG	5.13	127.11	115.30
1	F	85	LEU	CB-CG-CD2	-5.07	102.37	111.00

There are no chirality outliers.

There are no planarity outliers.

## 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	994	0	957	12	0
1	B	993	0	949	20	0
1	C	993	0	949	11	0
1	D	989	0	946	7	0
1	E	1001	0	962	11	0
1	F	993	0	949	13	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
3	A	63	0	0	3	0
3	B	32	0	0	0	0
3	C	45	0	0	1	0
3	D	52	0	0	1	0
3	E	31	0	0	1	0
3	F	36	0	0	0	0
All	All	6228	0	5712	65	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 (65) 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:E:109:CYS:SG	3:E:208:HOH:O	2.39	0.80
1:C:3:LEU:HD12	1:C:49:ILE:HD12	1.64	0.79
1:D:104:ARG:HG3	1:D:114:GLU:HG3	1.69	0.73
1:D:114:GLU:OE2	1:D:116:ARG:NH2	2.22	0.72
1:D:107:GLU:HB3	3:D:250:HOH:O	1.89	0.71
1:C:3:LEU:CD1	1:C:49:ILE:HD12	2.20	0.71
1:B:102:LYS:HD2	1:B:114:GLU:CD	2.19	0.63
1:F:3:LEU:HG	1:F:49:ILE:HD12	1.81	0.63
1:F:7:PHE:CE2	1:F:36:ILE:HD12	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:THR:HG21	3:A:232:HOH:O	1.99	0.60
1:B:34:VAL:HA	1:B:104:ARG:O	2.00	0.60
1:F:94:LYS:NZ	1:F:98:PRO:O	2.30	0.60
1:D:37:HIS:HB2	1:D:102:LYS:HB3	1.83	0.59
1:A:-1:SER:O	1:B:118:ASP:O	2.20	0.59
1:C:38:ILE:HD13	1:C:55:ILE:HD11	1.84	0.58
1:B:60:LYS:HG2	1:B:64:GLU:OE2	2.04	0.58
1:B:37:HIS:HB2	1:B:102:LYS:HB3	1.86	0.58
1:B:62:ILE:CD1	1:B:93:LEU:HD13	2.33	0.57
1:A:37:HIS:HB2	1:A:102:LYS:HB3	1.86	0.57
1:E:88:TRP:O	1:E:92:GLN:HG2	2.06	0.56
1:E:104:ARG:HG3	1:E:114:GLU:HG3	1.88	0.55
1:E:30:HIS:CD2	1:E:107:GLU:HG2	2.43	0.54
1:F:43:ASP:HB3	1:F:46:THR:OG1	2.08	0.53
1:B:38:ILE:HD13	1:B:55:ILE:HD11	1.89	0.53
1:A:87:ARG:HH22	1:C:-1:SER:HB2	1.73	0.53
1:E:48:TRP:HB2	1:F:83:GLU:OE2	2.09	0.53
1:E:11:SER:HB3	1:E:71:LEU:HD13	1.91	0.52
1:B:33:ARG:NH2	1:B:109:CYS:HA	2.24	0.52
1:E:7:PHE:HE1	1:E:56:LYS:HG3	1.75	0.52
1:C:37:HIS:HB2	1:C:102:LYS:HB3	1.92	0.51
1:F:35:ALA:HB3	1:F:104:ARG:HB3	1.94	0.50
1:A:-1:SER:HB2	1:B:87:ARG:NH1	2.26	0.50
1:F:7:PHE:HE2	1:F:36:ILE:HD12	1.77	0.49
1:A:110:THR:O	1:C:5:LYS:HD2	2.13	0.48
1:B:11:SER:HB3	1:B:71:LEU:HD13	1.96	0.48
1:F:13:HIS:HB2	1:F:80:PRO:HG2	1.95	0.48
1:B:60:LYS:HB3	1:B:61:PRO:HD3	1.96	0.47
1:C:49:ILE:O	3:C:213:HOH:O	2.20	0.47
1:B:94:LYS:HA	1:B:94:LYS:HD2	1.64	0.47
1:A:87:ARG:NE	3:A:242:HOH:O	2.35	0.47
1:B:84:ASN:OD1	1:B:87:ARG:NH2	2.47	0.46
1:D:11:SER:HB3	1:D:71:LEU:HD13	1.96	0.46
1:D:102:LYS:HD2	1:D:114:GLU:OE2	2.16	0.46
1:F:3:LEU:HD12	1:F:38:ILE:HD11	1.98	0.46
1:E:-1:SER:OG	1:F:87:ARG:HD3	2.15	0.46
1:A:113:CYS:HB2	1:C:3:LEU:HD23	1.98	0.46
1:B:9:PHE:HD2	1:B:11:SER:OG	2.01	0.44
1:B:50:ARG:HD2	1:B:99:GLU:OE2	2.18	0.44
1:F:9:PHE:HD2	1:F:11:SER:OG	2.00	0.44
1:F:1:MSE:HB2	1:F:49:ILE:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:PHE:CE1	1:C:112:GLY:HA3	2.54	0.43
1:A:102:LYS:HD2	1:A:114:GLU:CD	2.39	0.43
1:A:87:ARG:NH2	3:A:242:HOH:O	2.44	0.42
1:B:4:PHE:HA	1:B:36:ILE:O	2.19	0.42
1:E:34:VAL:HA	1:E:104:ARG:O	2.18	0.42
1:B:15:LEU:HD12	1:B:24:CYS:HB3	2.02	0.42
1:D:42:VAL:HG22	1:E:83:GLU:HG2	2.02	0.42
1:C:51:ASP:HB3	1:C:54:GLU:HG3	2.02	0.42
1:A:7:PHE:HE2	1:A:36[A]:ILE:HD12	1.85	0.41
1:C:33:ARG:NH2	1:C:109:CYS:HA	2.35	0.41
1:E:37:HIS:HB2	1:E:102:LYS:HB3	2.02	0.41
1:A:102:LYS:HD2	1:A:114:GLU:CG	2.50	0.41
1:F:88:TRP:O	1:F:92:GLN:HG2	2.20	0.41
1:B:3:LEU:HD13	1:B:49:ILE:HD12	2.03	0.40
1:B:1:MSE:HB2	1:B:49:ILE:HD11	2.03	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	119/138 (86%)	116 (98%)	3 (2%)	0	100	100
1	B	119/138 (86%)	119 (100%)	0	0	100	100
1	C	119/138 (86%)	117 (98%)	2 (2%)	0	100	100
1	D	118/138 (86%)	116 (98%)	2 (2%)	0	100	100
1	E	120/138 (87%)	117 (98%)	3 (2%)	0	100	100
1	F	119/138 (86%)	117 (98%)	2 (2%)	0	100	100
All	All	714/828 (86%)	702 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	109/121 (90%)	100 (92%)	9 (8%)	13	13
1	B	108/121 (89%)	99 (92%)	9 (8%)	13	13
1	C	108/121 (89%)	104 (96%)	4 (4%)	39	49
1	D	108/121 (89%)	101 (94%)	7 (6%)	20	22
1	E	109/121 (90%)	103 (94%)	6 (6%)	25	30
1	F	108/121 (89%)	105 (97%)	3 (3%)	49	60
All	All	650/726 (90%)	612 (94%)	38 (6%)	23	27

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	SER
1	A	3	LEU
1	A	13	HIS
1	A	42	VAL
1	A	48	TRP
1	A	71	LEU
1	A	82	SER
1	A	99	GLU
1	A	105	VAL
1	B	3	LEU
1	B	13	HIS
1	B	42	VAL
1	B	48	TRP
1	B	66	LEU
1	B	71	LEU
1	B	82	SER
1	B	85	LEU
1	B	92	GLN
1	C	13	HIS
1	C	48	TRP
1	C	71	LEU
1	C	93	LEU

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Mol	Chain	Res	Type
1	D	3	LEU
1	D	13	HIS
1	D	20	GLU
1	D	48	TRP
1	D	71	LEU
1	D	93	LEU
1	D	105	VAL
1	E	13	HIS
1	E	14	ARG
1	E	20	GLU
1	E	48	TRP
1	E	71	LEU
1	E	82	SER
1	F	13	HIS
1	F	48	TRP
1	F	64	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	119/138 (86%)	0.27	6 (5%) 30 41	39, 45, 54, 58	0
1	B	120/138 (86%)	0.13	5 (4%) 37 48	39, 45, 53, 57	0
1	C	120/138 (86%)	0.11	3 (2%) 58 67	39, 45, 52, 58	0
1	D	119/138 (86%)	0.33	6 (5%) 30 41	39, 45, 53, 60	0
1	E	120/138 (86%)	0.31	8 (6%) 19 27	40, 45, 54, 61	0
1	F	120/138 (86%)	0.14	6 (5%) 30 41	39, 45, 54, 62	0
All	All	718/828 (86%)	0.21	34 (4%) 32 43	39, 45, 54, 62	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-2	GLY	5.0
1	A	45	HIS	4.6
1	E	-2	GLY	4.1
1	F	-2	GLY	3.8
1	E	0	HIS	3.6
1	E	-1	SER	3.5
1	E	21	GLY	3.4
1	B	-1	SER	3.2
1	C	118	ASP	3.1
1	A	20	GLU	3.0
1	F	20	GLU	3.0
1	B	20	GLU	2.9
1	E	45	HIS	2.8
1	A	109	CYS	2.8
1	E	118	ASP	2.7
1	F	118	ASP	2.7
1	F	16	PRO	2.7
1	D	118	ASP	2.6
1	D	-1	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	21	GLY	2.5
1	D	109	CYS	2.5
1	D	45	HIS	2.5
1	A	-1	SER	2.4
1	B	118	ASP	2.2
1	C	109	CYS	2.2
1	C	110	THR	2.2
1	A	110	THR	2.1
1	A	21	GLY	2.1
1	F	22	HIS	2.1
1	E	44	PRO	2.1
1	D	34	VAL	2.1
1	D	0	HIS	2.1
1	E	20	GLU	2.1
1	B	87	ARG	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ZN	F	200	1/1	0.98	0.03	-3.33	56,56,56,56	0
2	ZN	D	200	1/1	0.99	0.02	-4.05	42,42,42,42	0
2	ZN	C	200	1/1	0.99	0.02	-4.99	50,50,50,50	0
2	ZN	E	200	1/1	0.97	0.04	-6.84	53,53,53,53	0
2	ZN	B	200	1/1	0.99	0.02	-8.29	54,54,54,54	0
2	ZN	A	200	1/1	1.00	0.02	-	37,37,37,37	0

## 6.5 Other polymers

There are no such residues in this entry.