



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 05:08 AM GMT

PDB ID : 4EXB  
Title : Putative aldo-keto reductase from *Pseudomonas aeruginosa*  
Authors : Schnell, R.; Schneider, G.; Sandalova, T.  
Deposited on : 2012-04-30  
Resolution : 2.75 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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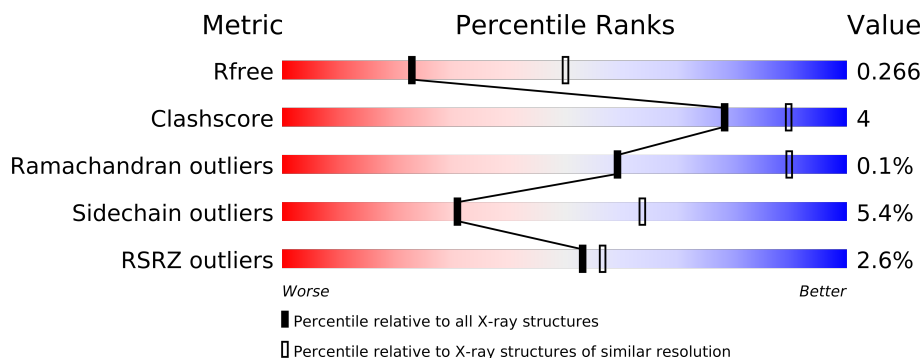
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.75 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))
$R_{free}$	66092	2406 (2.80-2.72)
Clashscore	79885	2995 (2.80-2.72)
Ramachandran outliers	78287	2941 (2.80-2.72)
Sidechain outliers	78261	2944 (2.80-2.72)
RSRZ outliers	66119	2409 (2.80-2.72)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	292	
1	B	292	
1	C	292	
1	D	292	
1	E	292	
1	F	292	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11681 atoms, of which 0 are hydrogen and 0 are deuterium.

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	253	Total	C	N	O	S	0	0	0
			1926	1204	352	366	4			
1	B	255	Total	C	N	O	S	0	0	0
			1946	1220	356	366	4			
1	C	250	Total	C	N	O	S	0	0	0
			1900	1191	348	357	4			
1	D	255	Total	C	N	O	S	0	0	0
			1948	1223	354	367	4			
1	E	255	Total	C	N	O	S	0	0	0
			1944	1218	354	368	4			
1	F	251	Total	C	N	O	S	0	0	0
			1910	1196	350	360	4			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	EXPRESSION TAG	UNP Q9HUH3
A	-20	HIS	-	EXPRESSION TAG	UNP Q9HUH3
A	-19	HIS	-	EXPRESSION TAG	UNP Q9HUH3
A	-18	HIS	-	EXPRESSION TAG	UNP Q9HUH3
A	-17	HIS	-	EXPRESSION TAG	UNP Q9HUH3
A	-16	HIS	-	EXPRESSION TAG	UNP Q9HUH3
A	-15	HIS	-	EXPRESSION TAG	UNP Q9HUH3
A	-14	SER	-	EXPRESSION TAG	UNP Q9HUH3
A	-13	SER	-	EXPRESSION TAG	UNP Q9HUH3
A	-12	GLY	-	EXPRESSION TAG	UNP Q9HUH3
A	-11	VAL	-	EXPRESSION TAG	UNP Q9HUH3
A	-10	ASP	-	EXPRESSION TAG	UNP Q9HUH3
A	-9	LEU	-	EXPRESSION TAG	UNP Q9HUH3
A	-8	GLY	-	EXPRESSION TAG	UNP Q9HUH3
A	-7	THR	-	EXPRESSION TAG	UNP Q9HUH3
A	-6	GLU	-	EXPRESSION TAG	UNP Q9HUH3
A	-5	ASN	-	EXPRESSION TAG	UNP Q9HUH3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	LEU	-	EXPRESSION TAG	UNP Q9HUH3
A	-3	TYR	-	EXPRESSION TAG	UNP Q9HUH3
A	-2	PHE	-	EXPRESSION TAG	UNP Q9HUH3
A	-1	GLN	-	EXPRESSION TAG	UNP Q9HUH3
A	0	SER	-	EXPRESSION TAG	UNP Q9HUH3
B	-21	MET	-	EXPRESSION TAG	UNP Q9HUH3
B	-20	HIS	-	EXPRESSION TAG	UNP Q9HUH3
B	-19	HIS	-	EXPRESSION TAG	UNP Q9HUH3
B	-18	HIS	-	EXPRESSION TAG	UNP Q9HUH3
B	-17	HIS	-	EXPRESSION TAG	UNP Q9HUH3
B	-16	HIS	-	EXPRESSION TAG	UNP Q9HUH3
B	-15	HIS	-	EXPRESSION TAG	UNP Q9HUH3
B	-14	SER	-	EXPRESSION TAG	UNP Q9HUH3
B	-13	SER	-	EXPRESSION TAG	UNP Q9HUH3
B	-12	GLY	-	EXPRESSION TAG	UNP Q9HUH3
B	-11	VAL	-	EXPRESSION TAG	UNP Q9HUH3
B	-10	ASP	-	EXPRESSION TAG	UNP Q9HUH3
B	-9	LEU	-	EXPRESSION TAG	UNP Q9HUH3
B	-8	GLY	-	EXPRESSION TAG	UNP Q9HUH3
B	-7	THR	-	EXPRESSION TAG	UNP Q9HUH3
B	-6	GLU	-	EXPRESSION TAG	UNP Q9HUH3
B	-5	ASN	-	EXPRESSION TAG	UNP Q9HUH3
B	-4	LEU	-	EXPRESSION TAG	UNP Q9HUH3
B	-3	TYR	-	EXPRESSION TAG	UNP Q9HUH3
B	-2	PHE	-	EXPRESSION TAG	UNP Q9HUH3
B	-1	GLN	-	EXPRESSION TAG	UNP Q9HUH3
B	0	SER	-	EXPRESSION TAG	UNP Q9HUH3
C	-21	MET	-	EXPRESSION TAG	UNP Q9HUH3
C	-20	HIS	-	EXPRESSION TAG	UNP Q9HUH3
C	-19	HIS	-	EXPRESSION TAG	UNP Q9HUH3
C	-18	HIS	-	EXPRESSION TAG	UNP Q9HUH3
C	-17	HIS	-	EXPRESSION TAG	UNP Q9HUH3
C	-16	HIS	-	EXPRESSION TAG	UNP Q9HUH3
C	-15	HIS	-	EXPRESSION TAG	UNP Q9HUH3
C	-14	SER	-	EXPRESSION TAG	UNP Q9HUH3
C	-13	SER	-	EXPRESSION TAG	UNP Q9HUH3
C	-12	GLY	-	EXPRESSION TAG	UNP Q9HUH3
C	-11	VAL	-	EXPRESSION TAG	UNP Q9HUH3
C	-10	ASP	-	EXPRESSION TAG	UNP Q9HUH3
C	-9	LEU	-	EXPRESSION TAG	UNP Q9HUH3
C	-8	GLY	-	EXPRESSION TAG	UNP Q9HUH3
C	-7	THR	-	EXPRESSION TAG	UNP Q9HUH3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	GLU	-	EXPRESSION TAG	UNP Q9HUH3
C	-5	ASN	-	EXPRESSION TAG	UNP Q9HUH3
C	-4	LEU	-	EXPRESSION TAG	UNP Q9HUH3
C	-3	TYR	-	EXPRESSION TAG	UNP Q9HUH3
C	-2	PHE	-	EXPRESSION TAG	UNP Q9HUH3
C	-1	GLN	-	EXPRESSION TAG	UNP Q9HUH3
C	0	SER	-	EXPRESSION TAG	UNP Q9HUH3
D	-21	MET	-	EXPRESSION TAG	UNP Q9HUH3
D	-20	HIS	-	EXPRESSION TAG	UNP Q9HUH3
D	-19	HIS	-	EXPRESSION TAG	UNP Q9HUH3
D	-18	HIS	-	EXPRESSION TAG	UNP Q9HUH3
D	-17	HIS	-	EXPRESSION TAG	UNP Q9HUH3
D	-16	HIS	-	EXPRESSION TAG	UNP Q9HUH3
D	-15	HIS	-	EXPRESSION TAG	UNP Q9HUH3
D	-14	SER	-	EXPRESSION TAG	UNP Q9HUH3
D	-13	SER	-	EXPRESSION TAG	UNP Q9HUH3
D	-12	GLY	-	EXPRESSION TAG	UNP Q9HUH3
D	-11	VAL	-	EXPRESSION TAG	UNP Q9HUH3
D	-10	ASP	-	EXPRESSION TAG	UNP Q9HUH3
D	-9	LEU	-	EXPRESSION TAG	UNP Q9HUH3
D	-8	GLY	-	EXPRESSION TAG	UNP Q9HUH3
D	-7	THR	-	EXPRESSION TAG	UNP Q9HUH3
D	-6	GLU	-	EXPRESSION TAG	UNP Q9HUH3
D	-5	ASN	-	EXPRESSION TAG	UNP Q9HUH3
D	-4	LEU	-	EXPRESSION TAG	UNP Q9HUH3
D	-3	TYR	-	EXPRESSION TAG	UNP Q9HUH3
D	-2	PHE	-	EXPRESSION TAG	UNP Q9HUH3
D	-1	GLN	-	EXPRESSION TAG	UNP Q9HUH3
D	0	SER	-	EXPRESSION TAG	UNP Q9HUH3
E	-21	MET	-	EXPRESSION TAG	UNP Q9HUH3
E	-20	HIS	-	EXPRESSION TAG	UNP Q9HUH3
E	-19	HIS	-	EXPRESSION TAG	UNP Q9HUH3
E	-18	HIS	-	EXPRESSION TAG	UNP Q9HUH3
E	-17	HIS	-	EXPRESSION TAG	UNP Q9HUH3
E	-16	HIS	-	EXPRESSION TAG	UNP Q9HUH3
E	-15	HIS	-	EXPRESSION TAG	UNP Q9HUH3
E	-14	SER	-	EXPRESSION TAG	UNP Q9HUH3
E	-13	SER	-	EXPRESSION TAG	UNP Q9HUH3
E	-12	GLY	-	EXPRESSION TAG	UNP Q9HUH3
E	-11	VAL	-	EXPRESSION TAG	UNP Q9HUH3
E	-10	ASP	-	EXPRESSION TAG	UNP Q9HUH3
E	-9	LEU	-	EXPRESSION TAG	UNP Q9HUH3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-8	GLY	-	EXPRESSION TAG	UNP Q9HUH3
E	-7	THR	-	EXPRESSION TAG	UNP Q9HUH3
E	-6	GLU	-	EXPRESSION TAG	UNP Q9HUH3
E	-5	ASN	-	EXPRESSION TAG	UNP Q9HUH3
E	-4	LEU	-	EXPRESSION TAG	UNP Q9HUH3
E	-3	TYR	-	EXPRESSION TAG	UNP Q9HUH3
E	-2	PHE	-	EXPRESSION TAG	UNP Q9HUH3
E	-1	GLN	-	EXPRESSION TAG	UNP Q9HUH3
E	0	SER	-	EXPRESSION TAG	UNP Q9HUH3
F	-21	MET	-	EXPRESSION TAG	UNP Q9HUH3
F	-20	HIS	-	EXPRESSION TAG	UNP Q9HUH3
F	-19	HIS	-	EXPRESSION TAG	UNP Q9HUH3
F	-18	HIS	-	EXPRESSION TAG	UNP Q9HUH3
F	-17	HIS	-	EXPRESSION TAG	UNP Q9HUH3
F	-16	HIS	-	EXPRESSION TAG	UNP Q9HUH3
F	-15	HIS	-	EXPRESSION TAG	UNP Q9HUH3
F	-14	SER	-	EXPRESSION TAG	UNP Q9HUH3
F	-13	SER	-	EXPRESSION TAG	UNP Q9HUH3
F	-12	GLY	-	EXPRESSION TAG	UNP Q9HUH3
F	-11	VAL	-	EXPRESSION TAG	UNP Q9HUH3
F	-10	ASP	-	EXPRESSION TAG	UNP Q9HUH3
F	-9	LEU	-	EXPRESSION TAG	UNP Q9HUH3
F	-8	GLY	-	EXPRESSION TAG	UNP Q9HUH3
F	-7	THR	-	EXPRESSION TAG	UNP Q9HUH3
F	-6	GLU	-	EXPRESSION TAG	UNP Q9HUH3
F	-5	ASN	-	EXPRESSION TAG	UNP Q9HUH3
F	-4	LEU	-	EXPRESSION TAG	UNP Q9HUH3
F	-3	TYR	-	EXPRESSION TAG	UNP Q9HUH3
F	-2	PHE	-	EXPRESSION TAG	UNP Q9HUH3
F	-1	GLN	-	EXPRESSION TAG	UNP Q9HUH3
F	0	SER	-	EXPRESSION TAG	UNP Q9HUH3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	16	Total O 16 16	0	0
2	B	21	Total O 21 21	0	0
2	C	17	Total O 17 17	0	0
2	D	18	Total O 18 18	0	0

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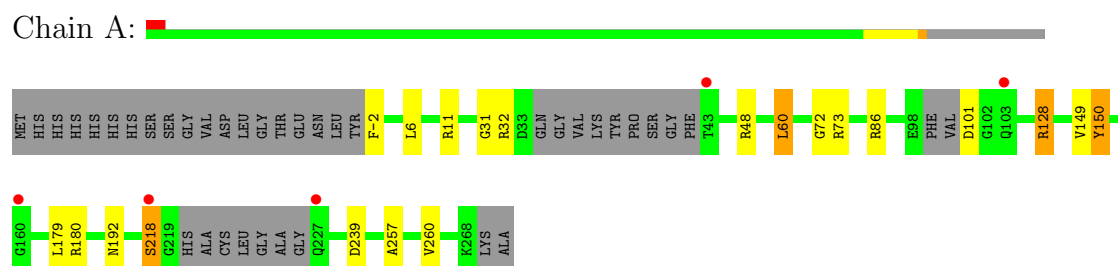
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	22	Total	O	0	0
			22	22		
2	F	13	Total	O	0	0
			13	13		

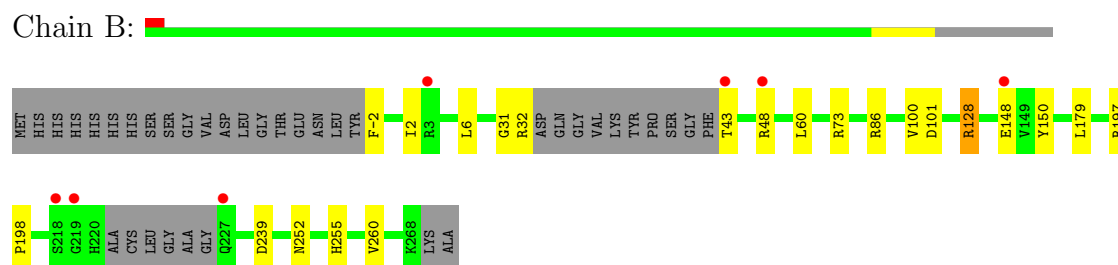
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

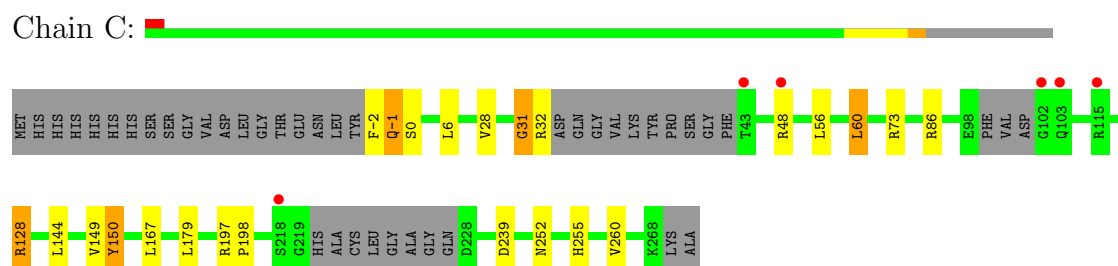
- Molecule 1: Putative uncharacterized protein



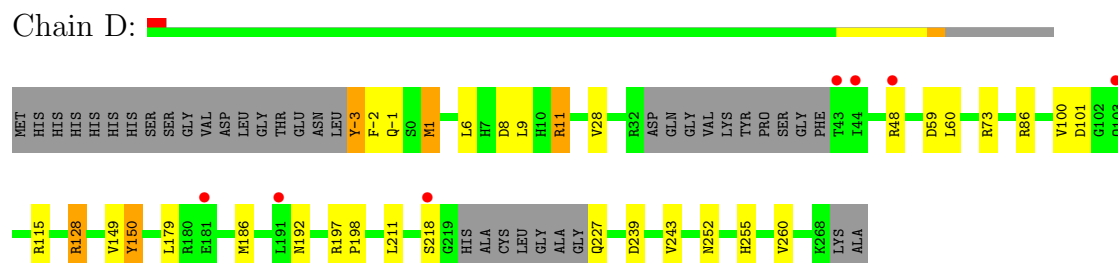
- Molecule 1: Putative uncharacterized protein



- Molecule 1: Putative uncharacterized protein



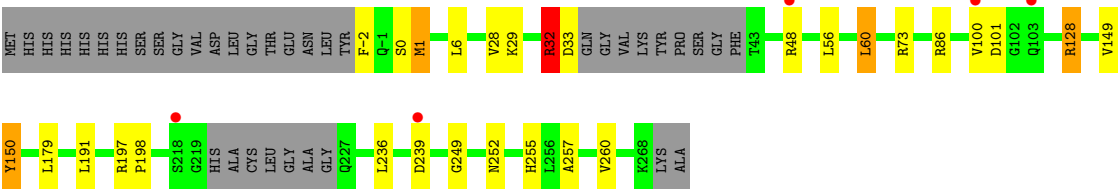
- Molecule 1: Putative uncharacterized protein





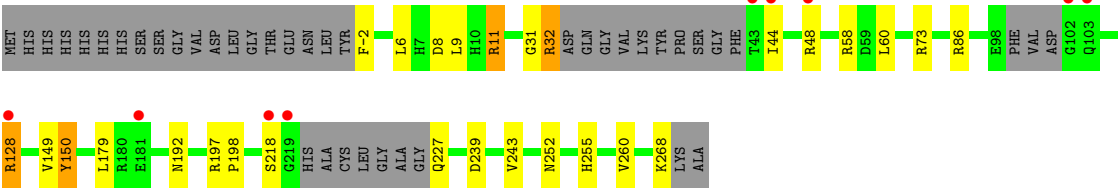
● Molecule 1: Putative uncharacterized protein

Chain E: 



● Molecule 1: Putative uncharacterized protein

Chain F: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.33Å 119.04Å 150.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.87 – 2.75 41.87 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.5 (41.87-2.75) 99.4 (41.87-2.75)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.243 , 0.274 0.238 , 0.266	Depositor DCC
$R_{free}$ test set	2250 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.9	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 13.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 44596 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11681	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.62	0/1953	0.68	0/2640
1	B	0.63	0/1976	0.70	0/2673
1	C	0.62	2/1927 (0.1%)	0.71	3/2605 (0.1%)
1	D	0.60	0/1978	0.70	0/2676
1	E	0.64	1/1973 (0.1%)	0.71	1/2669 (0.0%)
1	F	0.62	0/1937	0.70	0/2618
All	All	0.62	3/11744 (0.0%)	0.70	4/15881 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	28	VAL	CB-CG2	-5.57	1.41	1.52
1	C	28	VAL	CB-CG2	-5.17	1.42	1.52
1	C	73	ARG	CG-CD	-5.03	1.39	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	32	ARG	N-CA-C	6.20	127.73	111.00
1	C	-2	PHE	CB-CA-C	5.90	122.20	110.40
1	C	73	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	C	73	ARG	NE-CZ-NH1	-5.08	117.76	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1926	0	1940	11	0
1	B	1946	0	1959	8	0
1	C	1900	0	1921	9	0
1	D	1948	0	1964	18	0
1	E	1944	0	1959	22	0
1	F	1910	0	1932	18	0
2	A	16	0	0	2	0
2	B	21	0	0	2	0
2	C	17	0	0	0	0
2	D	18	0	0	3	0
2	E	22	0	0	1	0
2	F	13	0	0	3	0
All	All	11681	0	11675	83	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (83) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:148:GLU:HG3	2:B:303:HOH:O	1.63	0.98
1:E:32:ARG:O	1:E:32:ARG:HG3	1.78	0.83
1:F:32:ARG:HA	1:F:44:ILE:HG12	1.59	0.83
1:E:32:ARG:O	1:E:32:ARG:CG	2.32	0.77
1:F:32:ARG:CB	1:F:44:ILE:HD11	2.16	0.75
1:F:32:ARG:HB3	1:F:44:ILE:HD11	1.68	0.75
1:F:192:ASN:ND2	1:F:218:SER:HA	2.05	0.69
1:A:31:GLY:O	1:A:72:GLY:HA3	1.93	0.68
1:A:192:ASN:ND2	1:A:218:SER:HA	2.10	0.66
1:C:31:GLY:O	1:C:32:ARG:O	2.16	0.64
1:F:128:ARG:CZ	2:F:301:HOH:O	2.46	0.63
1:C:-1:GLN:HA	1:C:-1:GLN:HE21	1.66	0.60
1:A:32:ARG:HG3	1:A:32:ARG:O	2.02	0.60
1:F:31:GLY:O	1:F:32:ARG:HB3	2.05	0.56
1:B:128:ARG:O	1:B:128:ARG:HG3	1.94	0.56
1:D:59:ASP:OD2	1:E:-2:PHE:CE1	2.59	0.56
1:E:128:ARG:C	1:E:128:ARG:HD2	2.27	0.55
1:A:128:ARG:HD2	1:A:128:ARG:C	2.28	0.55
1:A:192:ASN:HD21	1:A:218:SER:HA	1.72	0.54
1:E:100:VAL:HG13	1:E:101:ASP:N	2.23	0.54
1:E:100:VAL:HG13	1:E:101:ASP:H	1.74	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:128:ARG:NH2	2:F:301:HOH:O	2.43	0.52
1:D:128:ARG:C	1:D:128:ARG:HD2	2.30	0.52
1:E:29:LYS:HE2	1:E:249:GLY:O	2.10	0.52
1:E:6:LEU:HG	1:E:260:VAL:HG13	1.91	0.52
1:B:31:GLY:O	1:B:32:ARG:C	2.48	0.52
1:E:252:ASN:HD22	1:E:255:HIS:CG	2.28	0.51
1:F:192:ASN:HD21	1:F:218:SER:HA	1.72	0.50
1:C:128:ARG:HD2	1:C:128:ARG:C	2.31	0.50
1:C:252:ASN:HD22	1:C:255:HIS:CG	2.30	0.50
1:F:32:ARG:HB2	1:F:44:ILE:HD11	1.93	0.50
1:B:100:VAL:HG12	1:B:101:ASP:N	2.26	0.49
1:F:58:ARG:NH2	2:F:303:HOH:O	2.44	0.49
1:B:252:ASN:HD22	1:B:255:HIS:CG	2.30	0.49
1:F:128:ARG:HD2	1:F:128:ARG:C	2.33	0.49
1:A:6:LEU:HG	1:A:260:VAL:HG13	1.94	0.49
1:F:8:ASP:O	1:F:9:LEU:HD12	2.13	0.49
1:D:115:ARG:NH1	2:D:305:HOH:O	2.36	0.48
1:F:6:LEU:HG	1:F:260:VAL:HG13	1.96	0.48
1:A:150:TYR:HB2	2:A:313:HOH:O	2.13	0.47
1:B:43:THR:HG23	2:B:312:HOH:O	2.14	0.46
1:D:-3:TYR:N	2:D:303:HOH:O	2.48	0.46
1:D:100:VAL:HG12	1:D:101:ASP:N	2.31	0.46
1:E:60:LEU:HD21	1:E:257:ALA:HA	1.98	0.46
1:A:60:LEU:HD21	1:A:257:ALA:HA	1.98	0.45
1:B:6:LEU:HG	1:B:260:VAL:HG13	1.98	0.45
1:F:252:ASN:HD22	1:F:255:HIS:CG	2.35	0.45
1:E:-2:PHE:C	1:E:0:SER:H	2.20	0.45
1:F:268:LYS:HB3	1:F:268:LYS:HE2	1.85	0.45
1:F:149:VAL:HG13	1:F:150:TYR:N	2.32	0.45
1:B:197:ARG:N	1:B:198:PRO:CD	2.81	0.44
1:C:6:LEU:HG	1:C:260:VAL:HG13	1.99	0.44
1:D:8:ASP:O	1:D:9:LEU:HD12	2.17	0.44
1:A:128:ARG:O	1:A:128:ARG:HD2	2.18	0.43
1:D:192:ASN:HD21	1:D:218:SER:C	2.22	0.43
1:E:149:VAL:HG13	1:E:150:TYR:N	2.33	0.43
1:D:28:VAL:HG23	1:D:28:VAL:H	1.44	0.43
1:C:144:LEU:HD11	1:C:167:LEU:HD22	2.00	0.43
1:E:32:ARG:O	1:E:32:ARG:CD	2.67	0.42
1:E:100:VAL:CG1	1:E:101:ASP:H	2.32	0.42
1:D:11:ARG:NH1	1:D:243:VAL:O	2.52	0.42
1:D:115:ARG:NH2	2:D:307:HOH:O	2.51	0.42
1:F:197:ARG:N	1:F:198:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:6:LEU:HG	1:D:260:VAL:HG13	2.00	0.42
1:D:197:ARG:N	1:D:198:PRO:CD	2.82	0.42
1:E:197:ARG:N	1:E:198:PRO:CD	2.82	0.42
1:F:11:ARG:NH1	1:F:243:VAL:O	2.52	0.42
1:D:-2:PHE:CD2	1:E:56:LEU:HD13	2.55	0.42
1:D:252:ASN:HD22	1:D:255:HIS:CG	2.39	0.41
1:E:101:ASP:HA	2:E:320:HOH:O	2.20	0.41
1:D:1:MET:HE1	1:E:1:MET:HE2	2.03	0.41
1:E:191:LEU:HD23	1:E:236:LEU:HD22	2.02	0.41
1:E:33:ASP:C	1:E:33:ASP:OD1	2.58	0.41
1:A:149:VAL:HG13	1:A:150:TYR:N	2.36	0.41
1:D:186:MET:HA	1:D:211:LEU:O	2.21	0.41
1:E:32:ARG:O	1:E:32:ARG:HD3	2.20	0.41
1:C:56:LEU:HG	1:C:60:LEU:HD22	2.03	0.41
1:C:149:VAL:HG13	1:C:150:TYR:N	2.36	0.40
1:E:100:VAL:CG1	1:E:101:ASP:N	2.84	0.40
1:C:197:ARG:N	1:C:198:PRO:CD	2.84	0.40
1:D:149:VAL:HG13	1:D:150:TYR:N	2.36	0.40
1:D:128:ARG:HD3	1:D:128:ARG:HH11	1.72	0.40
1:A:-2:PHE:HA	2:A:311:HOH:O	2.22	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	245/292 (84%)	237 (97%)	8 (3%)	0	100	100
1	B	249/292 (85%)	238 (96%)	10 (4%)	1 (0%)	43	79
1	C	242/292 (83%)	236 (98%)	5 (2%)	1 (0%)	43	79
1	D	249/292 (85%)	241 (97%)	8 (3%)	0	100	100
1	E	249/292 (85%)	238 (96%)	11 (4%)	0	100	100
1	F	243/292 (83%)	241 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1477/1752 (84%)	1431 (97%)	44 (3%)	2 (0%)	59 90

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	31	GLY
1	B	2	ILE

### 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	200/230 (87%)	188 (94%)	12 (6%)	27 58
1	B	201/230 (87%)	192 (96%)	9 (4%)	38 72
1	C	196/230 (85%)	187 (95%)	9 (5%)	37 71
1	D	202/230 (88%)	189 (94%)	13 (6%)	25 55
1	E	202/230 (88%)	192 (95%)	10 (5%)	34 68
1	F	198/230 (86%)	186 (94%)	12 (6%)	26 58
All	All	1199/1380 (87%)	1134 (95%)	65 (5%)	31 64

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	48	ARG
1	A	60	LEU
1	A	73	ARG
1	A	86	ARG
1	A	101	ASP
1	A	128	ARG
1	A	150	TYR
1	A	179	LEU
1	A	180	ARG
1	A	218	SER
1	A	239	ASP

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Mol	Chain	Res	Type
1	B	-2	PHE
1	B	48	ARG
1	B	60	LEU
1	B	73	ARG
1	B	86	ARG
1	B	128	ARG
1	B	150	TYR
1	B	179	LEU
1	B	239	ASP
1	C	-1	GLN
1	C	0	SER
1	C	48	ARG
1	C	60	LEU
1	C	86	ARG
1	C	128	ARG
1	C	150	TYR
1	C	179	LEU
1	C	239	ASP
1	D	-3	TYR
1	D	-1	GLN
1	D	1	MET
1	D	11	ARG
1	D	48	ARG
1	D	60	LEU
1	D	73	ARG
1	D	86	ARG
1	D	128	ARG
1	D	150	TYR
1	D	179	LEU
1	D	227	GLN
1	D	239	ASP
1	E	1	MET
1	E	32	ARG
1	E	48	ARG
1	E	60	LEU
1	E	73	ARG
1	E	86	ARG
1	E	128	ARG
1	E	150	TYR
1	E	179	LEU
1	E	239	ASP
1	F	-2	PHE

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Mol	Chain	Res	Type
1	F	11	ARG
1	F	32	ARG
1	F	48	ARG
1	F	60	LEU
1	F	73	ARG
1	F	86	ARG
1	F	128	ARG
1	F	150	TYR
1	F	179	LEU
1	F	227	GLN
1	F	239	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	ASN
1	B	192	ASN
1	B	252	ASN
1	C	-1	GLN
1	C	252	ASN
1	D	85	GLN
1	D	192	ASN
1	E	252	ASN
1	F	-1	GLN
1	F	192	ASN
1	F	252	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

## 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	253/292 (86%)	0.21	5 (1%) 62 65	26, 39, 57, 63	0
1	B	255/292 (87%)	0.19	7 (2%) 52 55	26, 39, 58, 66	0
1	C	250/292 (85%)	0.20	6 (2%) 56 59	26, 39, 57, 70	0
1	D	255/292 (87%)	0.27	7 (2%) 52 55	26, 39, 56, 63	0
1	E	255/292 (87%)	0.18	5 (1%) 62 65	26, 39, 56, 63	0
1	F	251/292 (85%)	0.25	9 (3%) 41 43	26, 39, 57, 66	0
All	All	1519/1752 (86%)	0.22	39 (2%) 53 57	26, 39, 57, 70	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	43	THR	6.0
1	C	102	GLY	5.4
1	D	218	SER	5.2
1	F	44	ILE	5.2
1	B	219	GLY	4.3
1	F	102	GLY	4.1
1	E	218	SER	4.1
1	F	219	GLY	3.7
1	F	43	THR	3.6
1	D	48	ARG	3.3
1	B	3	ARG	3.2
1	D	103	GLN	3.1
1	E	48	ARG	3.0
1	F	218	SER	2.9
1	E	100	VAL	2.8
1	F	128	ARG	2.8
1	D	43	THR	2.7
1	A	103	GLN	2.7
1	B	227	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	227	GLN	2.7
1	C	218	SER	2.7
1	C	43	THR	2.5
1	B	218	SER	2.5
1	F	48	ARG	2.5
1	E	103	GLN	2.5
1	E	239	ASP	2.4
1	A	218	SER	2.4
1	D	44	ILE	2.3
1	A	43	THR	2.3
1	C	48	ARG	2.3
1	D	191	LEU	2.2
1	B	48	ARG	2.1
1	F	181	GLU	2.1
1	C	115	ARG	2.1
1	A	160	GLY	2.1
1	C	103	GLN	2.1
1	F	103	GLN	2.1
1	D	181	GLU	2.1
1	B	148	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.