



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 09:40 am BST

PDB ID : 2FWR  
Title : Structure of Archaeoglobus Fulgidis XPB  
Authors : Fan, L.; Arvai, A.S.; Tainer, J.A.  
Deposited on : 2006-02-02  
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<https://www.wwpdb.org/validation/2017/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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

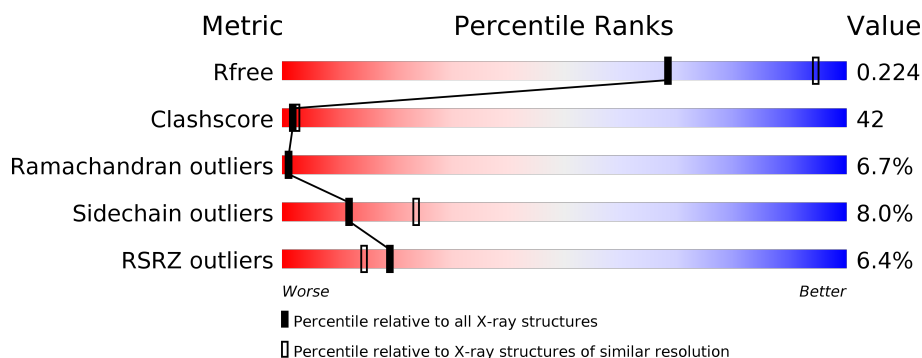
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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	472	<div> <div>7%</div> <div> <div>39%</div> <div>45%</div> <div>8%</div> <div>8%</div> </div> </div>
1	B	472	<div> <div>5%</div> <div> <div>43%</div> <div>40%</div> <div>6%</div> <div>10%</div> </div> </div>
1	C	472	<div> <div>4%</div> <div> <div>33%</div> <div>44%</div> <div>10%</div> <div>12%</div> </div> </div>
1	D	472	<div> <div>8%</div> <div> <div>31%</div> <div>50%</div> <div>10%</div> <div>9%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14769 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 DNA repair protein RAD25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	S	0	0	0
			3513	2242	627	638	6			
1	B	423	Total	C	N	O	S	0	0	0
			3419	2181	611	619	8			
1	C	414	Total	C	N	O	S	0	0	0
			3317	2119	589	604	5			
1	D	428	Total	C	N	O	S	0	0	0
			3402	2169	604	623	6			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP O29889
A	2	GLY	-	CLONING ARTIFACT	UNP O29889
A	3	SER	-	CLONING ARTIFACT	UNP O29889
A	4	SER	-	CLONING ARTIFACT	UNP O29889
A	5	HIS	-	EXPRESSION TAG	UNP O29889
A	6	HIS	-	EXPRESSION TAG	UNP O29889
A	7	HIS	-	EXPRESSION TAG	UNP O29889
A	8	HIS	-	EXPRESSION TAG	UNP O29889
A	9	HIS	-	EXPRESSION TAG	UNP O29889
A	10	HIS	-	EXPRESSION TAG	UNP O29889
A	11	SER	-	CLONING ARTIFACT	UNP O29889
A	12	SER	-	CLONING ARTIFACT	UNP O29889
A	13	GLY	-	CLONING ARTIFACT	UNP O29889
A	14	LEU	-	CLONING ARTIFACT	UNP O29889
A	15	VAL	-	CLONING ARTIFACT	UNP O29889
A	16	PRO	-	CLONING ARTIFACT	UNP O29889
A	17	ARG	-	CLONING ARTIFACT	UNP O29889
A	18	GLY	-	CLONING ARTIFACT	UNP O29889
A	19	SER	-	CLONING ARTIFACT	UNP O29889
A	20	HIS	-	CLONING ARTIFACT	UNP O29889
B	1	MET	-	INITIATING METHIONINE	UNP O29889

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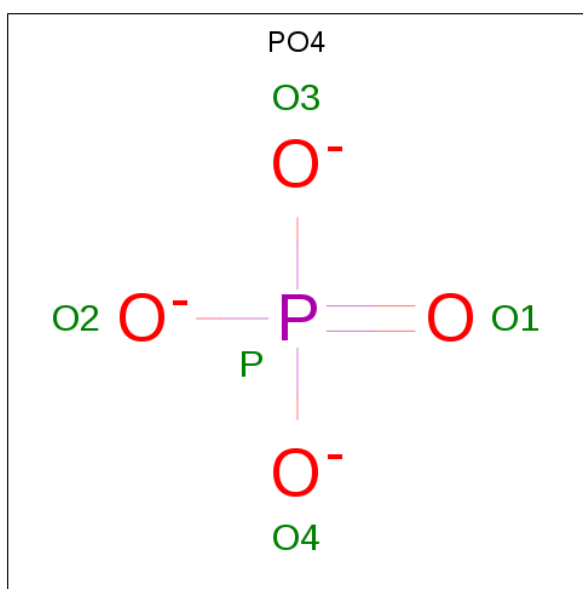
Chain	Residue	Modelled	Actual	Comment	Reference
B	2	GLY	-	CLONING ARTIFACT	UNP 029889
B	3	SER	-	CLONING ARTIFACT	UNP 029889
B	4	SER	-	CLONING ARTIFACT	UNP 029889
B	5	HIS	-	EXPRESSION TAG	UNP 029889
B	6	HIS	-	EXPRESSION TAG	UNP 029889
B	7	HIS	-	EXPRESSION TAG	UNP 029889
B	8	HIS	-	EXPRESSION TAG	UNP 029889
B	9	HIS	-	EXPRESSION TAG	UNP 029889
B	10	HIS	-	EXPRESSION TAG	UNP 029889
B	11	SER	-	CLONING ARTIFACT	UNP 029889
B	12	SER	-	CLONING ARTIFACT	UNP 029889
B	13	GLY	-	CLONING ARTIFACT	UNP 029889
B	14	LEU	-	CLONING ARTIFACT	UNP 029889
B	15	VAL	-	CLONING ARTIFACT	UNP 029889
B	16	PRO	-	CLONING ARTIFACT	UNP 029889
B	17	ARG	-	CLONING ARTIFACT	UNP 029889
B	18	GLY	-	CLONING ARTIFACT	UNP 029889
B	19	SER	-	CLONING ARTIFACT	UNP 029889
B	20	HIS	-	CLONING ARTIFACT	UNP 029889
C	1	MET	-	INITIATING METHIONINE	UNP 029889
C	2	GLY	-	CLONING ARTIFACT	UNP 029889
C	3	SER	-	CLONING ARTIFACT	UNP 029889
C	4	SER	-	CLONING ARTIFACT	UNP 029889
C	5	HIS	-	EXPRESSION TAG	UNP 029889
C	6	HIS	-	EXPRESSION TAG	UNP 029889
C	7	HIS	-	EXPRESSION TAG	UNP 029889
C	8	HIS	-	EXPRESSION TAG	UNP 029889
C	9	HIS	-	EXPRESSION TAG	UNP 029889
C	10	HIS	-	EXPRESSION TAG	UNP 029889
C	11	SER	-	CLONING ARTIFACT	UNP 029889
C	12	SER	-	CLONING ARTIFACT	UNP 029889
C	13	GLY	-	CLONING ARTIFACT	UNP 029889
C	14	LEU	-	CLONING ARTIFACT	UNP 029889
C	15	VAL	-	CLONING ARTIFACT	UNP 029889
C	16	PRO	-	CLONING ARTIFACT	UNP 029889
C	17	ARG	-	CLONING ARTIFACT	UNP 029889
C	18	GLY	-	CLONING ARTIFACT	UNP 029889
C	19	SER	-	CLONING ARTIFACT	UNP 029889
C	20	HIS	-	CLONING ARTIFACT	UNP 029889
D	1	MET	-	INITIATING METHIONINE	UNP 029889
D	2	GLY	-	CLONING ARTIFACT	UNP 029889
D	3	SER	-	CLONING ARTIFACT	UNP 029889

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Chain	Residue	Modelled	Actual	Comment	Reference
D	4	SER	-	CLONING ARTIFACT	UNP O29889
D	5	HIS	-	EXPRESSION TAG	UNP O29889
D	6	HIS	-	EXPRESSION TAG	UNP O29889
D	7	HIS	-	EXPRESSION TAG	UNP O29889
D	8	HIS	-	EXPRESSION TAG	UNP O29889
D	9	HIS	-	EXPRESSION TAG	UNP O29889
D	10	HIS	-	EXPRESSION TAG	UNP O29889
D	11	SER	-	CLONING ARTIFACT	UNP O29889
D	12	SER	-	CLONING ARTIFACT	UNP O29889
D	13	GLY	-	CLONING ARTIFACT	UNP O29889
D	14	LEU	-	CLONING ARTIFACT	UNP O29889
D	15	VAL	-	CLONING ARTIFACT	UNP O29889
D	16	PRO	-	CLONING ARTIFACT	UNP O29889
D	17	ARG	-	CLONING ARTIFACT	UNP O29889
D	18	GLY	-	CLONING ARTIFACT	UNP O29889
D	19	SER	-	CLONING ARTIFACT	UNP O29889
D	20	HIS	-	CLONING ARTIFACT	UNP O29889

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



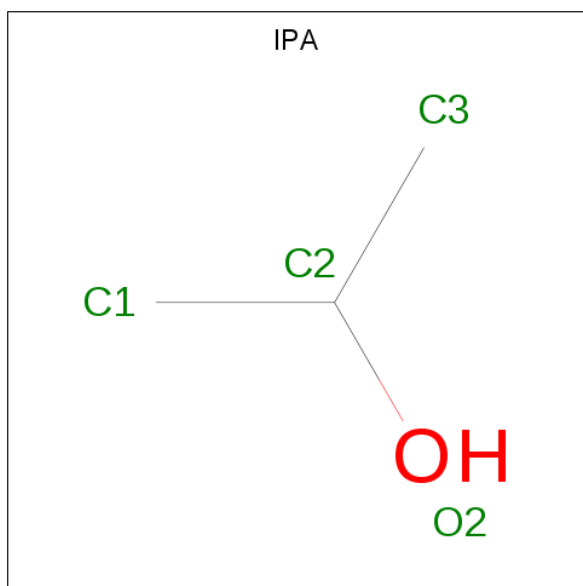
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C<sub>3</sub>H<sub>8</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	3	1		
3	A	1	Total	C	O	0	0
			4	3	1		
3	A	1	Total	C	O	0	0
			4	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	286	Total	O	0	0
			286	286		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	299	Total 299	O 299	0	0
4	C	261	Total 261	O 261	0	0
4	D	220	Total 220	O 220	0	0

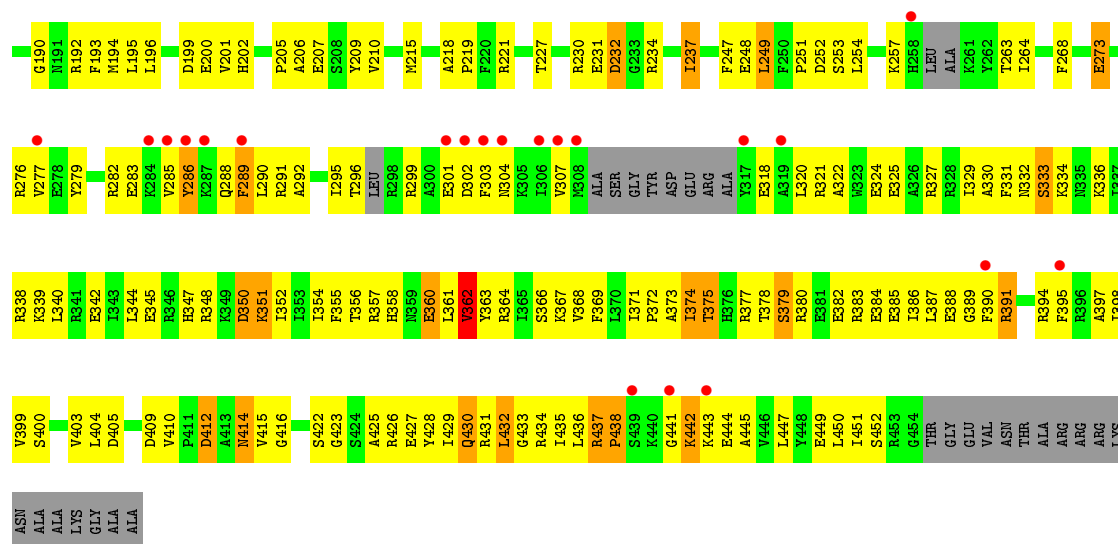
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ( $\text{RSRZ} > 2$ ). 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.

[illegible]

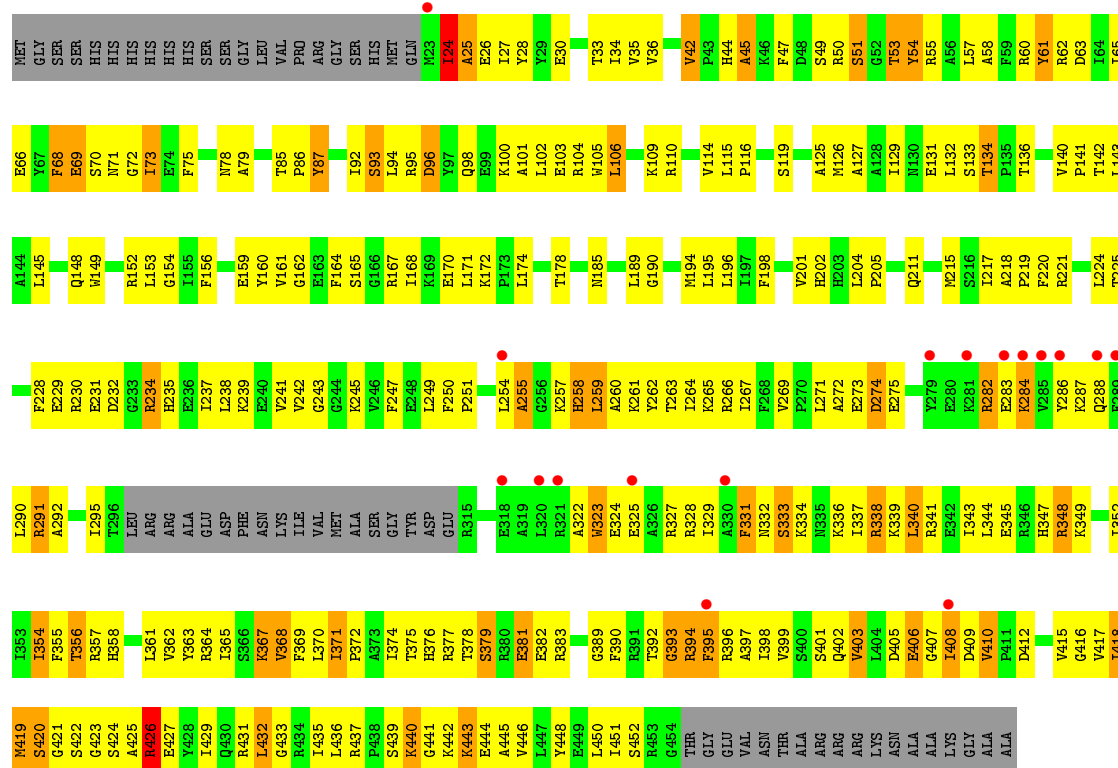
Chain B:

Amino Acid	Category
MET	Grey
GLY	Green
SER	Green
SER	Green
HIS	Green
HIS	Green
HIS	Green
HIS	Green
HIS	Green
SER	Green
SER	Green
SER	Green
LEU	Green
VAL	Green
PRO	Green
ARG	Green
ARG	Green
GLY	Green
HIS	Green
SER	Green
P21	Red
Q22	Yellow
P23	Yellow
I24	Yellow
E26	Yellow
I27	Yellow
Y28	Yellow
P31	Orange
I34	Yellow
V35	Yellow
V36	Yellow
K37	Yellow
G38	Yellow
P43	Yellow
H44	Yellow
A45	Yellow
D48	Yellow
S49	Yellow
R50	Yellow
T53	Yellow
Y54	Yellow
A58	Yellow
F59	Yellow
R60	Yellow
Y61	Yellow
R62	Yellow
D63	Yellow
E66	Yellow
Y67	Yellow
F68	Yellow
E69	Yellow
E70	Yellow
N71	Grey
G72	Green
F75	Green
A80	Green
D81	Green
P82	Green
F88	Green
I92	Green
S93	Green
E99	Green
K100	Green
A101	Green
L102	Green
E103	Green
R104	Green
W105	Green
L106	Green
R110	Green
L115	Green
S119	Green
G120	Green
K121	Green
T122	Green
M126	Green
M130	Green
S133	Green
T134	Green
L137	Green
L143	Green
E147	Green
Q148	Green
W149	Green
R152	Green
L153	Green
F156	Green
E163	Green
F164	Green
S165	Green
I168	Green
K169	Green
E187	Green

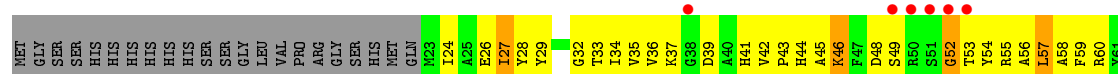




### • Molecule 1: DNA repair protein RAD25



### • Molecule 1: DNA repair protein RAD25



GLY	I408	R346	K284	S216	L137	R62
ALA	D409	H347	V285	I217	I138	D63
	V410		V286	A218	V139	I64
	P411	D350	K287	P219	V140	I65
		K351	K289	R221	P141	E66
	A413	I352	Q288	L222	T142	Y67
	N414	I353	L290		F68	F69
	V415	I354	R291		S70	
		F355	A292	T225	W149	
	V417	T356	R293	A226	K150	N71
	I418	R357	G294	T227	E151	G72
	M419	H358	I295	F228	R152	I73
	S420	N359	T296	E229	L153	E74
	G421	E360	LEU	R230	G154	F75
	G422	L361	ARG	E231	I155	V76
	G423	V362	ARG	D232		D77
	S424	R363	ALA	G233	E158	N78
	A425	R364	GLU	R234	A159	A79
	R426	I365	ASP		Y160	A80
	E427	S366	PHE	I237	V161	D81
	Y428	K367	ASN	L238	G162	P82
	I429	V368	K305	K239	E163	I83
	Q430	F369	I306		F164	P84
	R431	L370	V307	V242	S165	T85
	L432	I371	V308	G243	G166	P86
		P372	A309		R167	
	I435	A373	S310	V246	I168	E91
	L436	I374	G311		K169	I92
	R437	T375	V312	L249	E170	S93
	P438	H376	ASP	F250	L171	I94
	S439	R377	GLU	P251	K172	R95
	K440	T378	ARG	D252	P173	D86
	G441	S379	A316	S253	L174	Y97
	K442	R380	V317	L254	T175	Q98
	E443	E381	E318	A255	V176	E99
	E444	E382	A319	G256	S177	K100
		R383	L320	K257	T178	A101
	L447	E384	R321	H258	Y179	L102
	Y448		A322	L259	D180	
	E449	L387	K323	A260		W105
	L450	E388	E324	K261	V184	L106
	I451	G389	E325			
	R452	F390	A326	I264	M191	K109
	G453	R391	R327	K265	R192	R110
	T454	T392	K328	A266	F193	G111
	E455	G393	I329	I267	M194	C112
	G456	R394	A330	F268	L195	I113
	E457	F395	F331	V269		V114
	V458	R396	N332		F198	L115
	N459	A397	S333	E273		P116
	T460	I398		D274	V201	T117
	A461	V399	K336	E275		G118
	ARG	S400	I337	R276		
	ARG	S401	R338	V277	P205	K121
	ARG	Q402	K339	E278		
	LYS	V403	I340	Y279	V210	L132
	ASN	L404		E280		S133
	ALA	D405	T343	K281	A213	T134
	ALA	E406	I344	R282		P135
	LYS	G407	E345	E283	M215	T136

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.09 Å 97.96 Å 113.73 Å 79.03° 85.54° 89.69°	Depositor
Resolution (Å)	29.35 – 2.60 29.35 – 2.60	Depositor EDS
% Data completeness (in resolution range)	84.8 (29.35-2.60) 84.7 (29.35-2.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 2.61 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.237 , 0.300 0.211 , 0.224	Depositor DCC
$R_{free}$ test set	2888 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.5	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 102.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14769	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, IPA

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	0.49	0/3583	0.69	0/4827
1	B	0.48	0/3484	0.68	1/4688 (0.0%)
1	C	0.44	0/3383	0.67	0/4562
1	D	0.43	0/3466	0.65	0/4673
All	All	0.46	0/13916	0.67	1/18750 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	190	GLY	N-CA-C	5.20	126.10	113.10

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	3513	0	3546	303	0
1	B	3419	0	3446	243	0
1	C	3317	0	3324	302	0
1	D	3402	0	3401	310	0
2	A	5	0	0	0	0
2	B	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	0	0
2	D	15	0	0	0	0
3	A	12	0	24	6	0
4	A	286	0	0	14	1
4	B	299	0	0	10	3
4	C	261	0	0	12	0
4	D	220	0	0	12	1
All	All	14769	0	13741	1153	4

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 42.

The worst 5 of 1153 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:438:PRO:HB3	1:D:444:GLU:HA	1.31	1.08
1:A:333:SER:HB3	1:A:336:LYS:HG3	1.36	1.07
1:C:24:ILE:H	1:C:24:ILE:HD12	1.20	1.03
1:D:356:THR:HG23	1:D:362:VAL:HG22	1.38	1.01
1:D:95:ARG:HB3	1:D:259:LEU:HD11	1.39	1.01

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2319:HOH:O	4:B:2932:HOH:O[1_455]	1.98	0.22
4:B:2454:HOH:O	4:B:2522:HOH:O[1_655]	2.16	0.04
4:B:2433:HOH:O	4:B:2745:HOH:O[1_455]	2.18	0.02
4:D:2465:HOH:O	4:D:2580:HOH:O[1_655]	2.18	0.02

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	432/472 (92%)	343 (79%)	67 (16%)	22 (5%)	2	2
1	B	415/472 (88%)	341 (82%)	57 (14%)	17 (4%)	3	3
1	C	410/472 (87%)	304 (74%)	64 (16%)	42 (10%)	0	0
1	D	422/472 (89%)	313 (74%)	77 (18%)	32 (8%)	1	1
All	All	1679/1888 (89%)	1301 (78%)	265 (16%)	113 (7%)	1	1

5 of 113 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	259	LEU
1	A	297	LEU
1	A	307	VAL
1	A	313	ASP
1	A	331	PHE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	366/398 (92%)	333 (91%)	33 (9%)	9	18
1	B	357/398 (90%)	332 (93%)	25 (7%)	15	30
1	C	343/398 (86%)	323 (94%)	20 (6%)	20	40
1	D	349/398 (88%)	314 (90%)	35 (10%)	7	14
All	All	1415/1592 (89%)	1302 (92%)	113 (8%)	12	24

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	351	LYS
1	C	134	THR
1	D	392	THR
1	B	362	VAL
1	B	437	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	359	ASN
1	C	71	ASN
1	D	359	ASN
1	B	430	GLN
1	C	78	ASN

### 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 ⓘ

11 ligands are modelled in this entry.

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	$\# Z  > 2$
2	PO4	A	4001	-	4,4,4	1.66	1 (25%)	6,6,6	0.43	0
3	IPA	A	6002	-	3,3,3	0.42	0	3,3,3	0.37	0
2	PO4	B	4002	-	4,4,4	1.68	0	6,6,6	0.42	0
2	PO4	B	4008	-	4,4,4	1.65	1 (25%)	6,6,6	0.40	0
2	PO4	D	4005	-	4,4,4	1.64	0	6,6,6	0.43	0
2	PO4	C	4003	-	4,4,4	1.75	0	6,6,6	0.42	0
2	PO4	D	4006	-	4,4,4	1.61	0	6,6,6	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	IPA	A	6003	-	3,3,3	0.38	0	3,3,3	0.33	0
2	PO4	B	4007	-	4,4,4	1.71	0	6,6,6	0.42	0
2	PO4	D	4004	-	4,4,4	1.81	2 (50%)	6,6,6	0.43	0
3	IPA	A	6001	-	3,3,3	0.42	0	3,3,3	0.38	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4004	PO4	P-O4	-2.07	1.48	1.54
2	B	4008	PO4	P-O3	-2.05	1.48	1.54
2	A	4001	PO4	P-O2	-2.05	1.48	1.54
2	D	4004	PO4	P-O2	-2.02	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	6002	IPA	3	0
2	B	4002	PO4	1	0
3	A	6001	IPA	3	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	434/472 (91%)	0.06	31 (7%) 16 11	12, 46, 121, 131	0
1	B	423/472 (89%)	-0.03	23 (5%) 25 20	11, 47, 122, 129	0
1	C	414/472 (87%)	0.19	17 (4%) 37 30	19, 68, 120, 132	0
1	D	428/472 (90%)	0.27	37 (8%) 10 7	18, 70, 123, 131	0
All	All	1699/1888 (89%)	0.12	108 (6%) 19 14	11, 58, 122, 132	0

The worst 5 of 108 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	290	LEU	7.2
1	A	291	ARG	6.4
1	C	285	VAL	5.4
1	C	279	TYR	5.4
1	D	52	GLY	5.3

### 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PO4	A	4001	5/5	0.89	0.16	85,86,87,87	0
2	PO4	D	4005	5/5	0.89	0.23	113,114,114,114	0
2	PO4	B	4007	5/5	0.90	0.20	88,89,90,90	0
2	PO4	D	4006	5/5	0.91	0.16	75,75,76,77	0
2	PO4	B	4008	5/5	0.92	0.17	82,83,84,84	0
3	IPA	A	6003	4/4	0.94	0.19	58,59,59,60	0
3	IPA	A	6001	4/4	0.95	0.15	44,44,45,45	0
3	IPA	A	6002	4/4	0.96	0.10	40,41,41,41	0
2	PO4	D	4004	5/5	0.96	0.15	65,65,66,67	0
2	PO4	B	4002	5/5	0.96	0.12	64,67,67,68	0
2	PO4	C	4003	5/5	0.97	0.12	89,89,90,90	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.