wwPDB X-ray Structure Validation Summary Report (i)

Feb 6, 2024 – 04:32 PM EST

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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

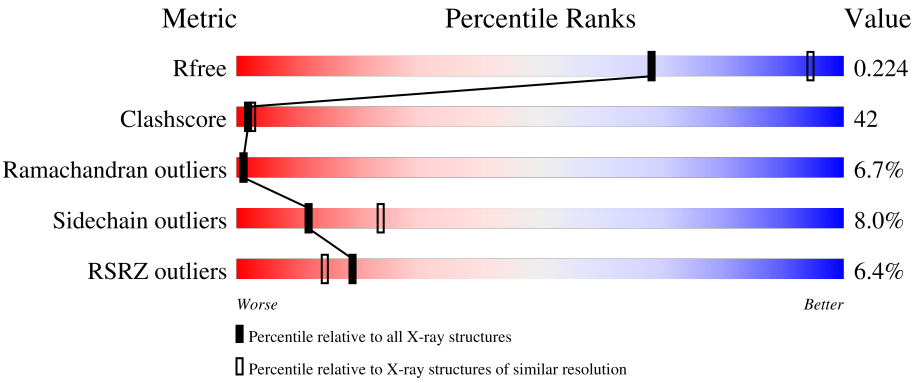
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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 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 <=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	7% 39% 45% 8% 8%
1	B	472	5% 43% 40% 6% 10%
1	C	472	4% 33% 44% 10% 12%
1	D	472	8% 31% 50% 10% 9%

2 Entry composition (i)

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 O29889
B	3	SER	-	cloning artifact	UNP O29889
B	4	SER	-	cloning artifact	UNP O29889
B	5	HIS	-	expression tag	UNP O29889
B	6	HIS	-	expression tag	UNP O29889
B	7	HIS	-	expression tag	UNP O29889
B	8	HIS	-	expression tag	UNP O29889
B	9	HIS	-	expression tag	UNP O29889
B	10	HIS	-	expression tag	UNP O29889
B	11	SER	-	cloning artifact	UNP O29889
B	12	SER	-	cloning artifact	UNP O29889
B	13	GLY	-	cloning artifact	UNP O29889
B	14	LEU	-	cloning artifact	UNP O29889
B	15	VAL	-	cloning artifact	UNP O29889
B	16	PRO	-	cloning artifact	UNP O29889
B	17	ARG	-	cloning artifact	UNP O29889
B	18	GLY	-	cloning artifact	UNP O29889
B	19	SER	-	cloning artifact	UNP O29889
B	20	HIS	-	cloning artifact	UNP O29889
C	1	MET	-	initiating methionine	UNP O29889
C	2	GLY	-	cloning artifact	UNP O29889
C	3	SER	-	cloning artifact	UNP O29889
C	4	SER	-	cloning artifact	UNP O29889
C	5	HIS	-	expression tag	UNP O29889
C	6	HIS	-	expression tag	UNP O29889
C	7	HIS	-	expression tag	UNP O29889
C	8	HIS	-	expression tag	UNP O29889
C	9	HIS	-	expression tag	UNP O29889
C	10	HIS	-	expression tag	UNP O29889
C	11	SER	-	cloning artifact	UNP O29889
C	12	SER	-	cloning artifact	UNP O29889
C	13	GLY	-	cloning artifact	UNP O29889
C	14	LEU	-	cloning artifact	UNP O29889
C	15	VAL	-	cloning artifact	UNP O29889
C	16	PRO	-	cloning artifact	UNP O29889
C	17	ARG	-	cloning artifact	UNP O29889
C	18	GLY	-	cloning artifact	UNP O29889
C	19	SER	-	cloning artifact	UNP O29889
C	20	HIS	-	cloning artifact	UNP O29889
D	1	MET	-	initiating methionine	UNP O29889
D	2	GLY	-	cloning artifact	UNP O29889
D	3	SER	-	cloning artifact	UNP O29889

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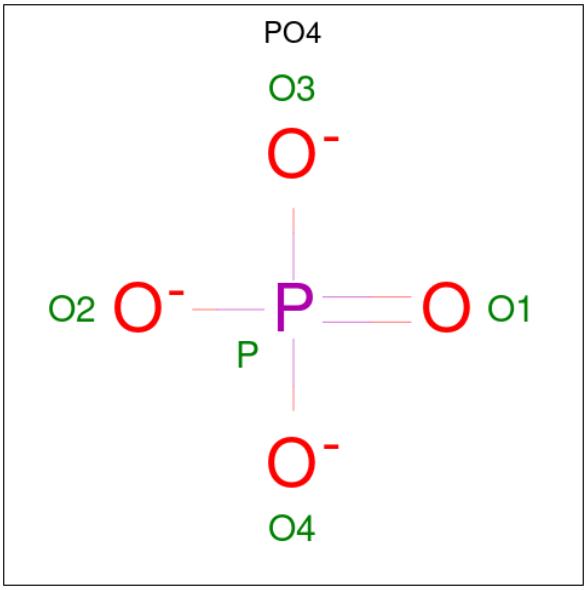
Chain	Residue	Modelled	Actual	Comment	Reference
D	4	SER	-	cloning artifact	UNP O29889
D	5	HIS	-	expression tag	UNP O29889
D	6	HIS	-	expression tag	UNP O29889
D	7	HIS	-	expression tag	UNP O29889
D	8	HIS	-	expression tag	UNP O29889
D	9	HIS	-	expression tag	UNP O29889
D	10	HIS	-	expression tag	UNP O29889
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_4P).



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

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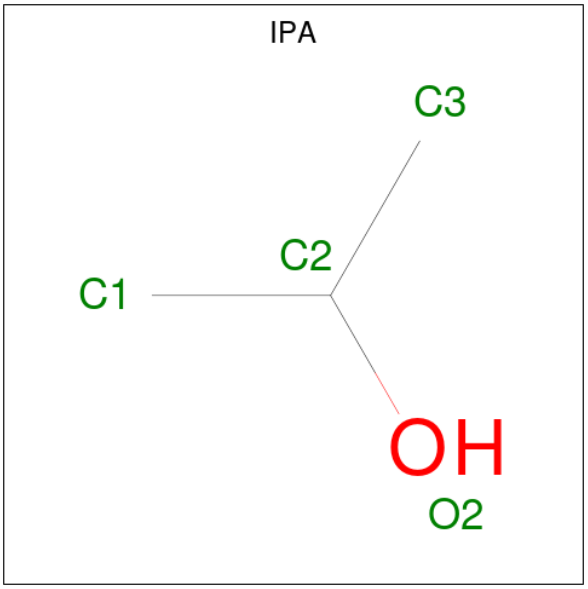
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0

- Molecule 3 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



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

- Molecule 4 is water.

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

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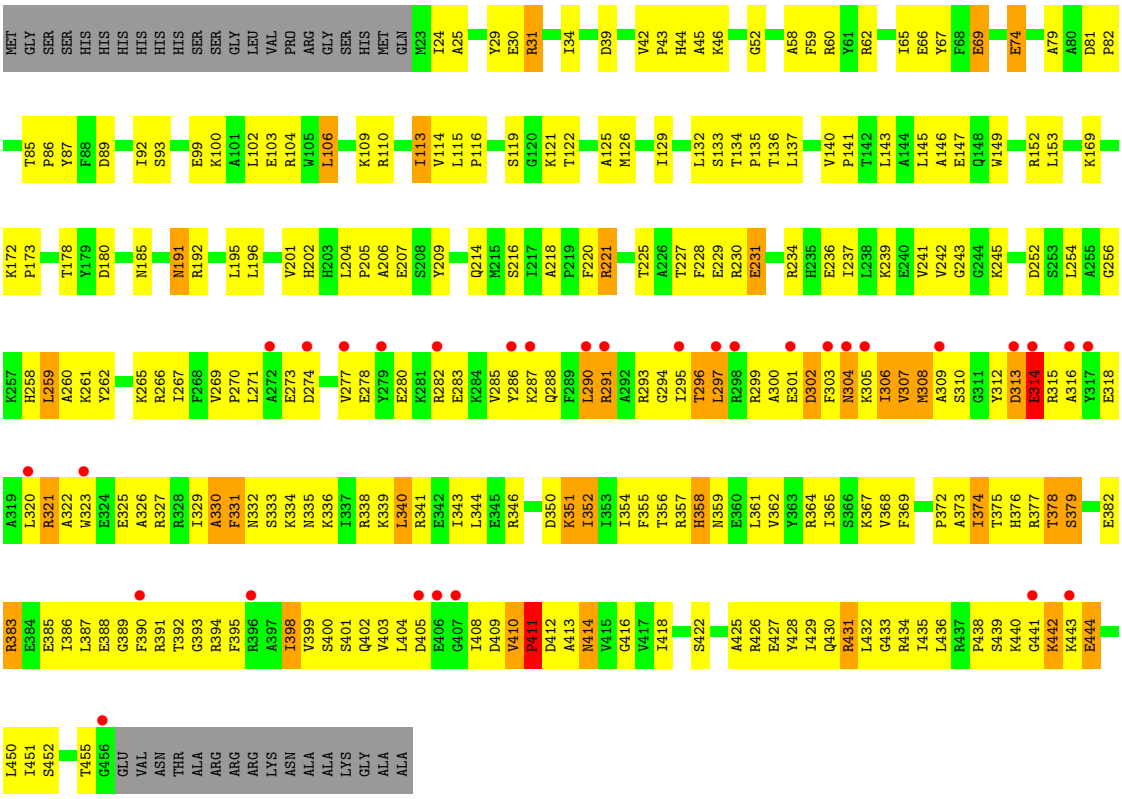
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	299	Total O 299 299	0	0
4	C	261	Total O 261 261	0	0
4	D	220	Total O 220 220	0	0

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.

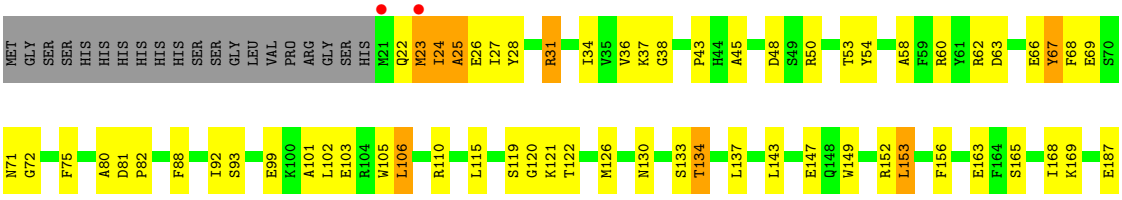
• Molecule 1: DNA repair protein RAD25

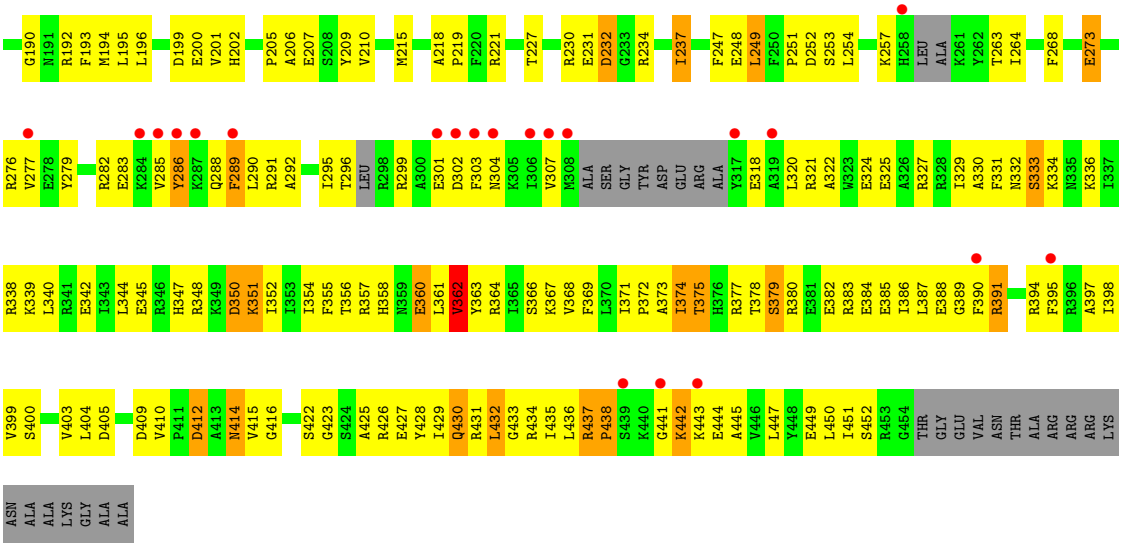
Chain A:



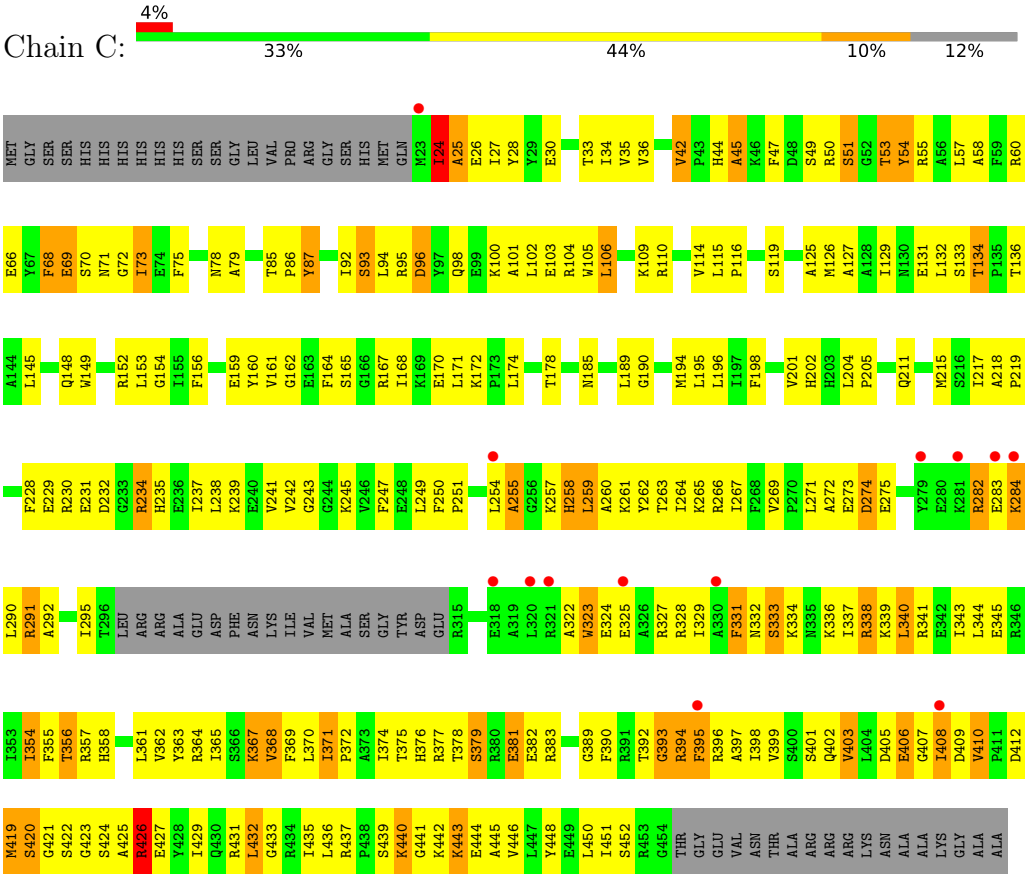
• Molecule 1: DNA repair protein RAD25

Chain B:

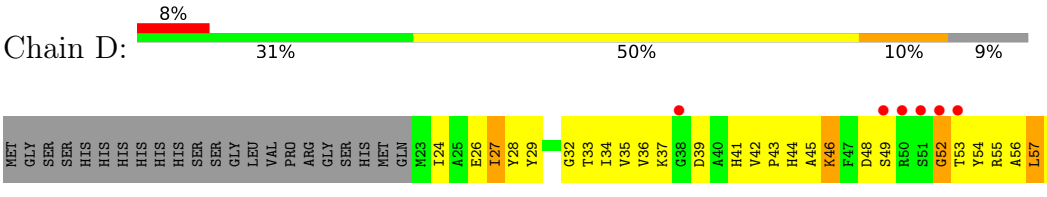


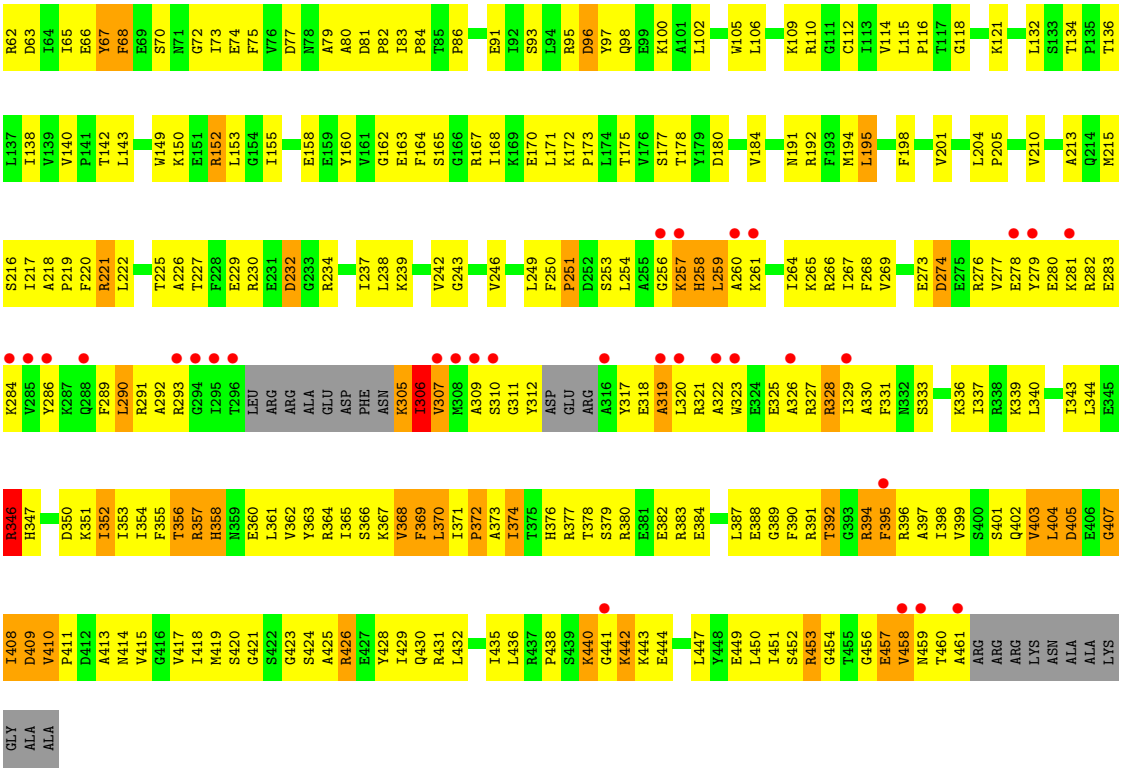


• Molecule 1: DNA repair protein RAD25



• Molecule 1: DNA repair protein RAD25




R62 D63 I64 I65 E66 Y67 F68 E69 S70 N71 G72 I73 E74 F75 V76 D77 N78 A79 A80 D81 P82 I83 P84 T85 P86 E91 I92 S93 L94 R95 D96 Y97 Q98 E99 K100 A101 L102 W105 L106 K109 R110 G111 C112 I113 V114 L115 P116 T117 G118 K121 L132 S133 T134 P135 T136
L137 I138 V139 V140 P141 T142 L143 W149 K150 E151 R152 L153 G154 I155 E158 E159 Y160 V161 G162 E163 F164 S165 G166 R167 I168 K169 E170 L171 K172 P173 L174 T175 V176 S177 T178 Y179 D180 V184 N191 R192 F193 M194 L195 F198 V201 L204 P205 V210 A213 Q214 M215
S216 I217 A218 P219 F220 R221 L222 T225 A226 T227 F228 E229 R230 E231 D232 G233 R234 I237 L238 K239 V242 G243 V246 L249 F250 P251 D252 S253 L254 A255 G256 K257 H258 L259 A260 K261 I264 K265 R266 I267 F268 V269 E273 D274 E275 R276 V277 E278 Y279 E280 K281 R282 E283
K284 V285 Y286 K287 Q288 F289 L290 R291 A292 R293 G294 I295 T296 LEU ARG ARG ALA GLU ASP PHE ASN K305 I306 V307 M308 A309 S310 G311 Y312 ASP GLU ARG A316 Y317 E318 A319 L320 R321 A322 W323 E324 E325 A326 R327 R328 I329 A330 F331 N332 S333 K336 I337 R338 K339 L340 I343 L344 E345
R346 H347 D350 K351 I352 I353 I354 F355 T356 R357 H358 N359 E360 L361 V362 V363 R364 I365 S366 K367 V368 F369 L370 I371 P372 A373 I374 T375 H376 R377 T378 S379 R380 E381 E382 R383 E384 L387 E388 G389 F390 R391 T392 G393 R394 F395 R396 A397 I398 V399 S400 S401 Q402 V403 L404 D405 E406 G407
I408 D409 V410 P411 D412 A413 N414 V415 G416 V417 I418 M419 S420 G421 S422 G423 S424 A425 R426 E427 Y428 I429 Q430 R431 L432 I435 L436 R437 P438 S439 K440 G441 K442 K443 E444 L447 Y448 E449 L450 I451 S452 R453 G454 T455 G456 E457 V458 N459 T460 A461 ARG ARG ARG LYS ASN ALA ALA LYS
GLY ALA ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	49.09Å 97.96Å 113.73Å 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
$< I/\sigma(I) >$ [1]	2.44 (at 2.61Å)	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^2)	47.5	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 102.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: IPA, PO4

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(^{o})	Ideal(^{o})
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

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:HD12	1:C:24:ILE:H	1.20	1.03
1:D:356:THR:HG23	1:D:362:VAL:HG22	1.38	1.01
1:A:377:ARG:HG3	1:A:378:THR:H	1.23	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 (i)

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	437	ARG
1	D	409	ASP
1	C	354	ILE
1	D	405	ASP
1	D	356	THR

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

Mol	Chain	Res	Type
1	C	78	ASN
1	C	332	ASN
1	D	402	GLN
1	C	185	ASN
1	C	402	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	D	4006	-	4,4,4	1.61	0	6,6,6	0.48	0
3	IPA	A	6003	-	3,3,3	0.38	0	3,3,3	0.33	0
2	PO4	C	4003	-	4,4,4	1.75	0	6,6,6	0.42	0
2	PO4	A	4001	-	4,4,4	1.66	1 (25%)	6,6,6	0.43	0
2	PO4	D	4004	-	4,4,4	1.81	2 (50%)	6,6,6	0.43	0
2	PO4	B	4007	-	4,4,4	1.71	0	6,6,6	0.42	0
2	PO4	D	4005	-	4,4,4	1.64	0	6,6,6	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	IPA	A	6002	-	3,3,3	0.42	0	3,3,3	0.37	0
2	PO4	B	4008	-	4,4,4	1.65	1 (25%)	6,6,6	0.40	0
3	IPA	A	6001	-	3,3,3	0.42	0	3,3,3	0.38	0
2	PO4	B	4002	-	4,4,4	1.68	0	6,6,6	0.42	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
3	A	6001	IPA	3	0
2	B	4002	PO4	1	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, 95^{th} 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	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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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^{th} 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(Å^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
2	PO4	B	4002	5/5	0.96	0.12	64,67,67,68	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	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.