



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:11 AM GMT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

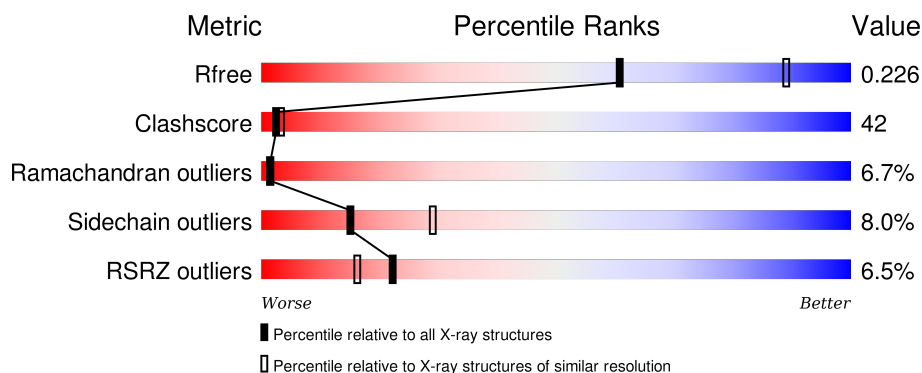
1 Overall quality at a glance ⓘ

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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 ≥ 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	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>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	B	4007	-	-	-	X
2	PO4	D	4005	-	-	-	X
2	PO4	D	4006	-	-	-	X

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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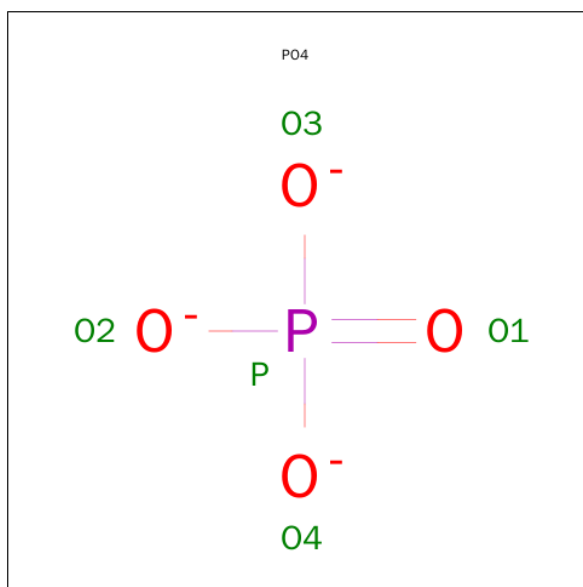
Chain	Residue	Modelled	Actual	Comment	Reference
B	2	GLY	-	CLONING ARTIFACT	UNP O29889
B	3	SER	-	CLONING ARTIFACT	UNP O29889
B	4	SER	-	CLONING ARTIFACT	UNP O29889
B	5	HIS	-	EXPRESSION TAG	UNP O29889
B	6	HIS	-	EXPRESSION TAG	UNP O29889
B	7	HIS	-	EXPRESSION TAG	UNP O29889
B	8	HIS	-	EXPRESSION TAG	UNP O29889
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: O₄P).



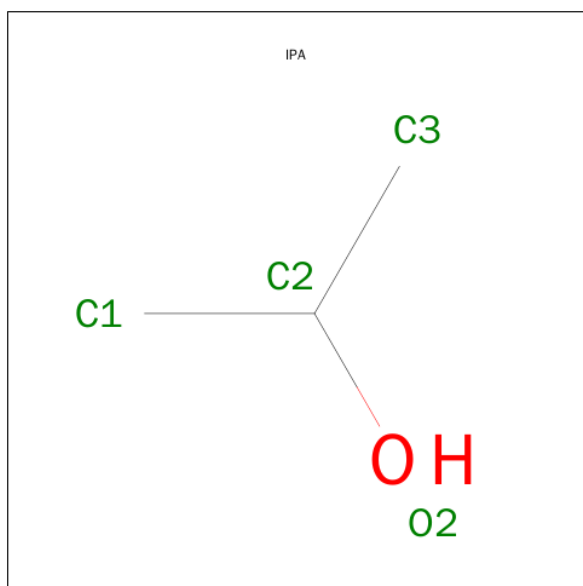
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		

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

- Molecule 3 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



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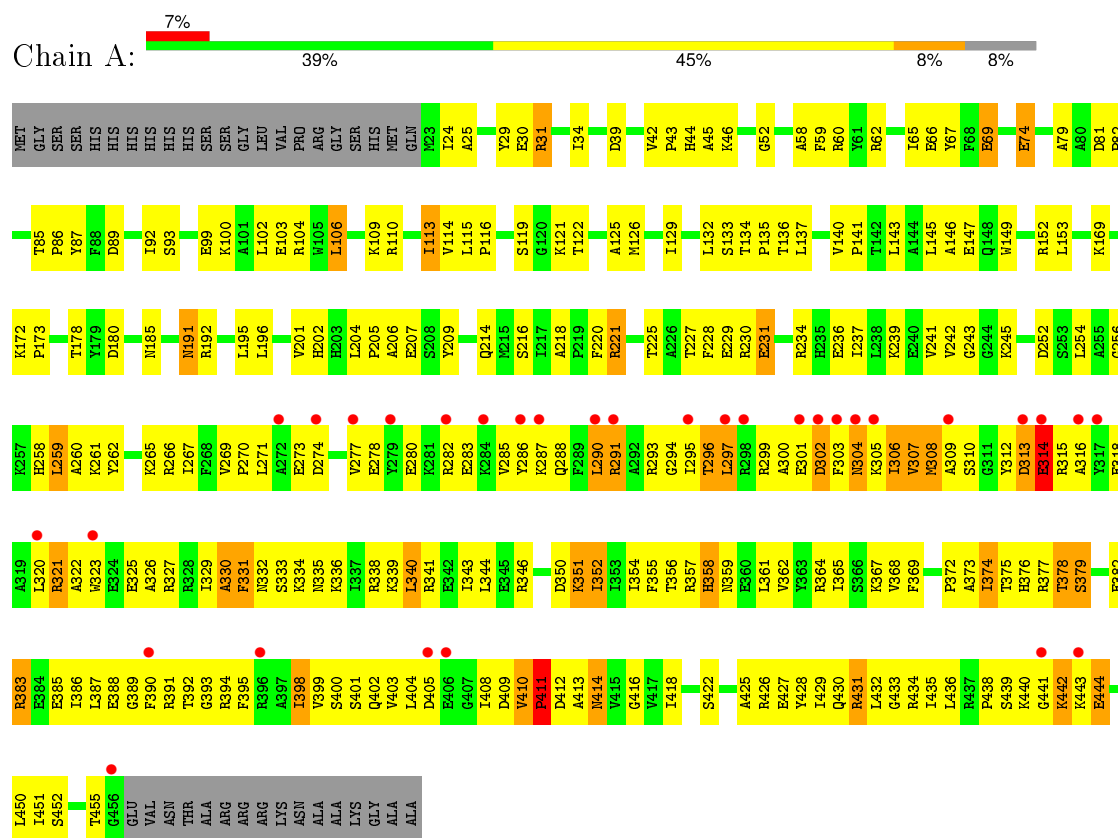
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	299	Total 299	O 299	0	0
4	C	261	Total 261	O 261	0	0
4	D	220	Total 220	O 220	0	0

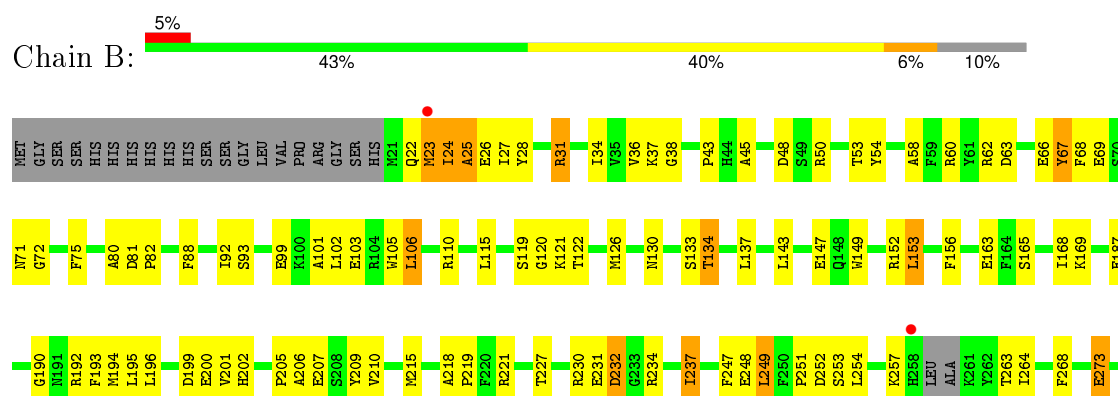
3 Residue-property plots

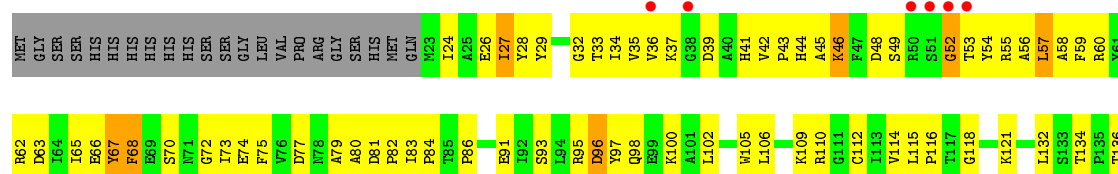
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: DNA repair protein RAD25



• Molecule 1: DNA repair protein RAD25





GLY	I408	K284	R346	L137
ALA	D409	V285	R347	I138
ALA	V410	Y286		V139
	P411	K287	D350	V140
	D412	K288	K351	F220
	A413	F289	I352	T142
	M414	L290	I353	P141
	V415	K291	I354	L143
	G416	A292	F355	
	V417	R293	T356	W149
	I418	G294	R357	K150
	M419	I295	R358	E151
	S420	T296	K359	R152
	G421	LEU	E360	L153
	G422	ARG	L361	G154
	S423	ARG	V362	I155
	S424	ALA	V363	E158
	A425	GLU	R364	E159
	R426	ASP	I365	Y160
	E427	PHE	S366	V161
	Y428	ASN	K367	G162
	I429	K305	V368	G163
	Q430	I306	F369	F164
	R431	V307	L370	S165
	L432	K308	I371	G166
		A309	P372	R167
	I435	S310	A373	I168
	L436	G311	I374	K169
	R437	Y312	T375	E170
	P438	ASP	R376	L171
	S439	GLU	R377	K172
	K440	ARG	T378	P173
	G441	A316	S379	L174
	R442	Y317	R380	T175
	K443	E318	E381	V176
	E444	A319	E382	S177
		L320	R383	T178
	L447	R321	E384	V179
	T448	K322		D180
	E449	E324	L387	V184
	L450	E325	E388	
	I451	A326	G389	N191
	S452	R327	F390	R192
	R453	K328	R391	F193
	G454	I329	T392	M194
	T455	A330	R394	L195
	G456	F331	G395	
	E457	K332	F395	F198
	V458	S333	R396	
	M459		A397	
	T460	E273	I398	V201
	A461	D274	V399	
	ARG	E275	ARG	L204
	ARG	R276	S400	K265
	LYS	I337	S401	R266
	ASN	R338	Q402	I267
	ALA	K339	V403	F268
	LYS	L340	L404	V269
	ALA	E280	D405	
	LYS	I343	E406	E273
		L344	LYS	D274
		E283		E275
				L204
				P205
				V210
				A213
				Q214
				M215

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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) 83.8 (29.35-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.61 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.237 , 0.300 0.215 , 0.226	Depositor DCC
R_{free} test set	2735 reflections (5.06%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 57207 reflections	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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 ⓘ

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	432/472 (92%)	343 (79%)	67 (16%)	22 (5%)	2	3
1	B	415/472 (88%)	341 (82%)	57 (14%)	17 (4%)	3	4
1	C	410/472 (87%)	304 (74%)	64 (16%)	42 (10%)	1	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%)	12	23
1	B	357/398 (90%)	332 (93%)	25 (7%)	19	37
1	C	343/398 (86%)	323 (94%)	20 (6%)	25	49
1	D	349/398 (88%)	314 (90%)	35 (10%)	9	18
All	All	1415/1592 (89%)	1302 (92%)	113 (8%)	15	29

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 [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 carbohydrates 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	A	4001	-	4,4,4	1.13	0	6,6,6	0.27	0
3	IPA	A	6001	-	3,3,3	0.35	0	3,3,3	0.36	0
3	IPA	A	6002	-	3,3,3	0.36	0	3,3,3	0.35	0
3	IPA	A	6003	-	3,3,3	0.31	0	3,3,3	0.31	0
2	PO4	B	4002	-	4,4,4	1.14	0	6,6,6	0.27	0
2	PO4	B	4007	-	4,4,4	1.17	0	6,6,6	0.27	0
2	PO4	B	4008	-	4,4,4	1.12	0	6,6,6	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	C	4003	-	4,4,4	1.20	0	6,6,6	0.27	0
2	PO4	D	4004	-	4,4,4	1.25	0	6,6,6	0.27	0
2	PO4	D	4005	-	4,4,4	1.11	0	6,6,6	0.27	0
2	PO4	D	4006	-	4,4,4	1.08	0	6,6,6	0.28	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	A	4001	-	-	0/0/0/0	0/0/0/0
3	IPA	A	6001	-	-	0/0/0/0	0/0/0/0
3	IPA	A	6002	-	-	0/0/0/0	0/0/0/0
3	IPA	A	6003	-	-	0/0/0/0	0/0/0/0
2	PO4	B	4002	-	-	0/0/0/0	0/0/0/0
2	PO4	B	4007	-	-	0/0/0/0	0/0/0/0
2	PO4	B	4008	-	-	0/0/0/0	0/0/0/0
2	PO4	C	4003	-	-	0/0/0/0	0/0/0/0
2	PO4	D	4004	-	-	0/0/0/0	0/0/0/0
2	PO4	D	4005	-	-	0/0/0/0	0/0/0/0
2	PO4	D	4006	-	-	0/0/0/0	0/0/0/0

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.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	6001	IPA	3	0
3	A	6002	IPA	3	0
2	B	4002	PO4	1	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	434/472 (91%)	0.08	32 (7%) 17 12	12, 46, 121, 131	0
1	B	423/472 (89%)	0.00	22 (5%) 31 24	11, 47, 122, 129	0
1	C	414/472 (87%)	0.21	18 (4%) 39 31	19, 68, 120, 132	0
1	D	428/472 (90%)	0.29	38 (8%) 12 8	18, 70, 123, 131	0
All	All	1699/1888 (89%)	0.15	110 (6%) 22 16	11, 58, 122, 132	0

The worst 5 of 110 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	290	LEU	7.3
1	A	291	ARG	6.5
1	C	285	VAL	5.5
1	D	52	GLY	5.4
1	C	279	TYR	5.4

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, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	PO4	B	4007	5/5	0.91	0.19	3.94	88,89,90,90	0
2	PO4	D	4005	5/5	0.88	0.24	3.21	113,114,114,114	0
2	PO4	D	4006	5/5	0.91	0.16	2.35	75,75,76,77	0
3	IPA	A	6003	4/4	0.94	0.19	1.59	58,59,59,60	0
2	PO4	B	4008	5/5	0.92	0.17	0.94	82,83,84,84	0
2	PO4	A	4001	5/5	0.89	0.16	0.38	85,86,87,87	0
2	PO4	B	4002	5/5	0.96	0.13	0.12	64,67,67,68	0
2	PO4	D	4004	5/5	0.96	0.15	0.04	65,65,66,67	0
3	IPA	A	6001	4/4	0.96	0.14	-0.01	44,44,45,45	0
2	PO4	C	4003	5/5	0.97	0.12	-0.77	89,89,90,90	0
3	IPA	A	6002	4/4	0.96	0.11	-	40,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.