



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 19, 2023 – 11:49 PM EDT

PDB ID : 2FZL  
Title : Structure of C-terminal domain of Archaeoglobus fulgidus XPB  
Authors : Fan, L.; Arvai, A.S.; Tainer, J.A.  
Deposited on : 2006-02-09  
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

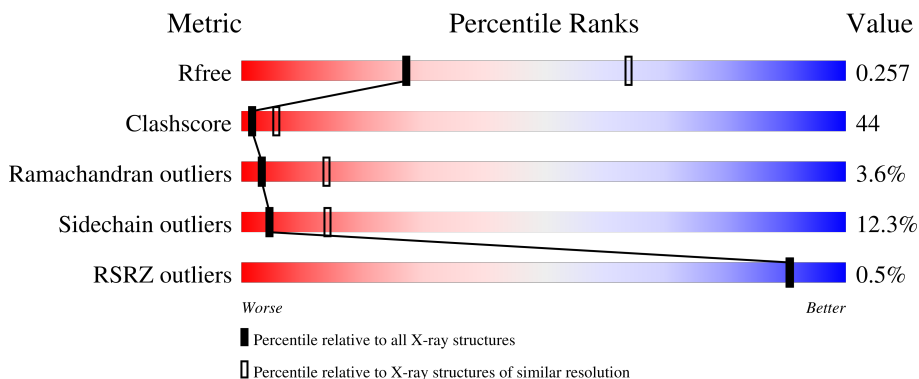
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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  $\geq 3$ , 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	219	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1665 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, XPB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	197	1638	1034	313	289	2	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	236	MET	-	initiating methionine	UNP O29889
A	237	GLY	-	cloning artifact	UNP O29889
A	238	SER	-	cloning artifact	UNP O29889
A	239	SER	-	cloning artifact	UNP O29889
A	240	HIS	-	expression tag	UNP O29889
A	241	HIS	-	expression tag	UNP O29889
A	242	HIS	-	expression tag	UNP O29889
A	243	HIS	-	expression tag	UNP O29889
A	244	HIS	-	expression tag	UNP O29889
A	245	HIS	-	expression tag	UNP O29889
A	246	SER	-	cloning artifact	UNP O29889
A	247	SER	-	cloning artifact	UNP O29889
A	248	GLY	-	cloning artifact	UNP O29889
A	249	LEU	-	cloning artifact	UNP O29889
A	250	VAL	-	cloning artifact	UNP O29889
A	251	PRO	-	cloning artifact	UNP O29889
A	252	ARG	-	cloning artifact	UNP O29889
A	253	GLY	-	cloning artifact	UNP O29889
A	254	SER	-	cloning artifact	UNP O29889
A	255	HIS	-	cloning artifact	UNP O29889
A	256	MET	-	cloning artifact	UNP O29889

- Molecule 2 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C<sub>3</sub>H<sub>8</sub>O).



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

- Molecule 3 is water.

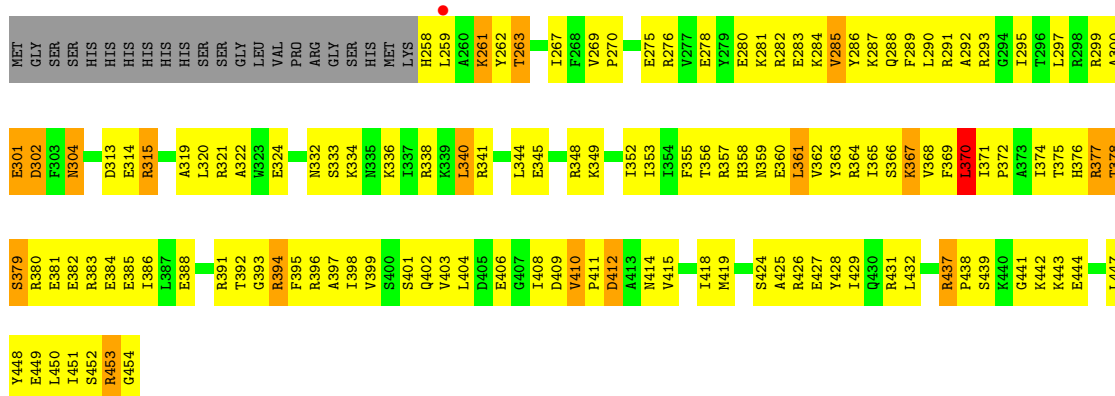
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	23	Total	O	0	0
			23	23		

### 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, XPB

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	172.86Å 172.86Å 172.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 49.90 – 2.91	Depositor EDS
% Data completeness (in resolution range)	92.4 (50.00-2.90) 92.6 (49.90-2.91)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.48 (at 2.91Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.249 , 0.291 0.243 , 0.257	Depositor DCC
$R_{free}$ test set	532 reflections (5.31%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	77.8	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 62.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	1665	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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: 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	0.50	0/1663	0.67	0/2222

There are no bond length outliers.

There are no bond angle outliers.

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	1638	0	1698	146	0
2	A	4	0	8	0	0
3	A	23	0	0	1	0
All	All	1665	0	1706	146	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 44.

All (146) 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:A:259:LEU:HD21	1:A:262:TYR:HB2	1.16	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:HIS:CE1	1:A:360:GLU:HB3	2.05	0.91
1:A:380:ARG:HE	1:A:383:ARG:HH22	1.14	0.91
1:A:332:ASN:HD22	1:A:364:ARG:HE	1.21	0.86
1:A:429:ILE:HD11	1:A:449:GLU:OE1	1.77	0.84
1:A:278:GLU:HG3	1:A:282:ARG:HH12	1.42	0.83
1:A:358:HIS:HE1	1:A:360:GLU:HB3	1.44	0.82
1:A:380:ARG:HE	1:A:383:ARG:NH2	1.75	0.82
1:A:304:ASN:HD22	1:A:304:ASN:N	1.74	0.82
1:A:424:SER:HA	1:A:449:GLU:OE2	1.81	0.80
1:A:379:SER:HB3	1:A:382:GLU:HB3	1.62	0.78
1:A:375:THR:HG22	1:A:378:THR:HG23	1.66	0.77
1:A:362:VAL:HG21	1:A:401:SER:HB3	1.66	0.76
1:A:374:ILE:HA	1:A:378:THR:HG21	1.69	0.75
1:A:269:VAL:O	1:A:452:SER:HA	1.88	0.73
1:A:284:LYS:O	1:A:288:GLN:HG3	1.89	0.72
1:A:442:LYS:HB3	1:A:444:GLU:HG3	1.72	0.70
1:A:437:ARG:HG3	1:A:438:PRO:HD2	1.74	0.70
1:A:349:LYS:HB2	1:A:349:LYS:NZ	2.07	0.69
1:A:261:LYS:HE3	1:A:263:THR:HG21	1.74	0.68
1:A:363:TYR:OH	1:A:375:THR:HG21	1.93	0.68
1:A:259:LEU:CD2	1:A:262:TYR:HB2	2.10	0.67
1:A:404:LEU:HA	1:A:408:ILE:HD12	1.75	0.66
1:A:282:ARG:HH11	1:A:282:ARG:HG2	1.60	0.66
1:A:438:PRO:HA	1:A:444:GLU:O	1.95	0.66
1:A:278:GLU:HG3	1:A:282:ARG:NH1	2.12	0.64
1:A:297:LEU:HD12	1:A:297:LEU:N	2.13	0.64
1:A:375:THR:H	1:A:378:THR:CG2	2.12	0.63
1:A:381:GLU:HG2	1:A:382:GLU:N	2.12	0.63
1:A:300:ALA:O	1:A:302:ASP:N	2.27	0.63
1:A:391:ARG:HB3	1:A:411:PRO:CG	2.28	0.63
1:A:403:VAL:HG21	1:A:431:ARG:HH12	1.63	0.62
1:A:380:ARG:O	1:A:384:GLU:HG3	1.99	0.62
1:A:288:GLN:HA	1:A:291:ARG:NH1	2.15	0.62
1:A:376:HIS:CE1	1:A:402:GLN:HB3	2.34	0.62
1:A:379:SER:HB3	1:A:382:GLU:CB	2.30	0.61
1:A:270:PRO:HB3	1:A:454:GLY:HA3	1.81	0.61
1:A:304:ASN:N	1:A:304:ASN:ND2	2.43	0.61
1:A:404:LEU:HB3	1:A:410:VAL:HG21	1.82	0.60
1:A:361:LEU:HD22	1:A:365:ILE:HG13	1.84	0.60
1:A:304:ASN:HD22	1:A:304:ASN:H	1.47	0.59
1:A:441:GLY:O	1:A:442:LYS:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:LEU:HD22	1:A:404:LEU:N	2.17	0.59
1:A:364:ARG:O	1:A:368:VAL:HG23	2.03	0.59
1:A:290:LEU:HD22	1:A:295:ILE:HB	1.85	0.58
1:A:304:ASN:ND2	1:A:304:ASN:H	2.02	0.58
1:A:396:ARG:HH11	1:A:396:ARG:HG2	1.70	0.57
1:A:375:THR:H	1:A:378:THR:HG23	1.69	0.57
1:A:391:ARG:HB3	1:A:411:PRO:HG3	1.86	0.56
1:A:393:GLY:O	1:A:395:PHE:N	2.38	0.56
1:A:453:ARG:HG2	1:A:454:GLY:N	2.20	0.56
1:A:419:MET:SD	1:A:450:LEU:HD12	2.46	0.56
1:A:375:THR:HA	1:A:401:SER:OG	2.06	0.56
1:A:301:GLU:H	1:A:304:ASN:ND2	2.04	0.55
1:A:362:VAL:HG13	1:A:399:VAL:HG22	1.87	0.55
1:A:259:LEU:HD12	1:A:438:PRO:HB3	1.89	0.55
1:A:283:GLU:O	1:A:287:LYS:HG3	2.08	0.54
1:A:374:ILE:HG22	1:A:402:GLN:HG2	1.88	0.54
1:A:425:ALA:O	1:A:429:ILE:HG13	2.07	0.54
1:A:378:THR:O	1:A:379:SER:HB2	2.06	0.54
1:A:364:ARG:HH11	1:A:364:ARG:HG3	1.72	0.54
1:A:278:GLU:CG	1:A:282:ARG:HH12	2.18	0.53
1:A:280:GLU:HA	1:A:283:GLU:HG2	1.90	0.53
1:A:404:LEU:O	1:A:408:ILE:HB	2.09	0.53
1:A:408:ILE:HG22	1:A:410:VAL:HG23	1.90	0.53
1:A:320:LEU:O	1:A:324:GLU:HG2	2.08	0.53
1:A:275:GLU:OE2	1:A:334:LYS:HG3	2.09	0.52
1:A:301:GLU:HA	1:A:304:ASN:CG	2.29	0.52
1:A:332:ASN:HD22	1:A:364:ARG:NE	1.99	0.52
1:A:369:PHE:O	1:A:371:ILE:N	2.41	0.52
1:A:340:LEU:HD22	1:A:344:LEU:HG	1.92	0.51
1:A:412:ASP:N	1:A:412:ASP:OD1	2.43	0.51
1:A:275:GLU:OE1	1:A:333:SER:HA	2.10	0.51
1:A:321:ARG:O	1:A:324:GLU:HB2	2.11	0.51
1:A:396:ARG:HG2	1:A:396:ARG:NH1	2.26	0.50
1:A:315:ARG:HH11	1:A:315:ARG:HG3	1.77	0.49
1:A:352:ILE:O	1:A:397:ALA:HA	2.13	0.49
1:A:278:GLU:O	1:A:281:LYS:HG2	2.12	0.49
1:A:261:LYS:HE3	1:A:263:THR:CG2	2.40	0.49
1:A:313:ASP:OD2	1:A:315:ARG:HB3	2.14	0.48
1:A:334:LYS:O	1:A:338:ARG:HG3	2.13	0.48
1:A:269:VAL:HG22	1:A:336:LYS:HE3	1.95	0.48
1:A:377:ARG:O	1:A:379:SER:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:PHE:CD2	1:A:356:THR:N	2.83	0.47
1:A:391:ARG:HG3	1:A:392:THR:HG23	1.95	0.47
1:A:333:SER:HB3	1:A:336:LYS:HG2	1.96	0.47
1:A:377:ARG:HB2	1:A:378:THR:H	1.44	0.47
1:A:297:LEU:N	1:A:297:LEU:CD1	2.77	0.47
1:A:267:ILE:HD11	1:A:448:TYR:HD2	1.79	0.46
1:A:357:ARG:HD2	1:A:428:TYR:OH	2.14	0.46
1:A:299:ARG:HA	1:A:299:ARG:HD3	1.71	0.46
1:A:300:ALA:C	1:A:302:ASP:H	2.15	0.46
1:A:447:LEU:C	1:A:447:LEU:HD23	2.36	0.46
1:A:375:THR:CG2	1:A:378:THR:HG23	2.42	0.46
1:A:382:GLU:O	1:A:385:GLU:HB3	2.14	0.46
1:A:300:ALA:O	1:A:301:GLU:HG2	2.16	0.46
1:A:364:ARG:O	1:A:367:LYS:HG3	2.15	0.46
1:A:372:PRO:HG2	1:A:395:PHE:CD2	2.51	0.46
1:A:388:GLU:OE1	1:A:388:GLU:HA	2.16	0.46
1:A:288:GLN:HG2	1:A:291:ARG:HH12	1.80	0.45
1:A:282:ARG:HG2	1:A:282:ARG:NH1	2.28	0.45
1:A:374:ILE:HD13	1:A:383:ARG:HG2	1.99	0.45
1:A:338:ARG:O	1:A:341:ARG:HB3	2.17	0.45
1:A:349:LYS:HB2	1:A:349:LYS:HZ2	1.80	0.45
1:A:366:SER:HB2	1:A:371:ILE:O	2.16	0.45
1:A:375:THR:H	1:A:378:THR:HG21	1.81	0.45
1:A:352:ILE:HG12	1:A:415:VAL:HB	1.99	0.45
1:A:403:VAL:C	1:A:404:LEU:HD22	2.38	0.45
1:A:259:LEU:CD1	1:A:438:PRO:HB3	2.46	0.44
1:A:367:LYS:HG3	1:A:368:VAL:N	2.31	0.44
1:A:403:VAL:HG21	1:A:431:ARG:NH1	2.30	0.44
1:A:319:ALA:O	1:A:322:ALA:HB3	2.17	0.44
1:A:349:LYS:HB2	1:A:349:LYS:HZ3	1.80	0.44
1:A:376:HIS:CE1	1:A:402:GLN:CB	3.01	0.44
1:A:382:GLU:O	1:A:386:ILE:HG13	2.18	0.44
1:A:375:THR:OG1	1:A:376:HIS:N	2.51	0.43
1:A:370:LEU:N	1:A:370:LEU:HD13	2.32	0.43
1:A:290:LEU:HA	1:A:290:LEU:HD23	1.71	0.43
1:A:402:GLN:O	1:A:404:LEU:HD22	2.18	0.43
1:A:438:PRO:HB2	1:A:443:LYS:HB3	2.01	0.43
1:A:289:PHE:HE2	1:A:315:ARG:HD2	1.83	0.43
1:A:403:VAL:CG2	1:A:431:ARG:NH1	2.82	0.43
1:A:449:GLU:OE2	1:A:451:ILE:HD11	2.18	0.43
1:A:371:ILE:CG2	1:A:398:ILE:HA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:GLY:O	1:A:394:ARG:HB2	2.19	0.43
1:A:301:GLU:HA	1:A:304:ASN:HB2	2.01	0.42
1:A:453:ARG:HG2	1:A:454:GLY:H	1.83	0.42
1:A:315:ARG:NH1	3:A:1007:HOH:O	2.52	0.42
1:A:406:GLU:O	1:A:408:ILE:N	2.51	0.42
1:A:313:ASP:O	1:A:314:GLU:C	2.58	0.42
1:A:341:ARG:O	1:A:345:GLU:HG3	2.20	0.42
1:A:419:MET:CE	1:A:450:LEU:HD12	2.50	0.42
1:A:382:GLU:O	1:A:383:ARG:C	2.58	0.42
1:A:301:GLU:HA	1:A:304:ASN:CB	2.50	0.41
1:A:352:ILE:HG22	1:A:353:ILE:N	2.34	0.41
1:A:361:LEU:CD2	1:A:365:ILE:HG13	2.48	0.41
1:A:409:ASP:O	1:A:410:VAL:O	2.38	0.41
1:A:427:GLU:HG2	1:A:431:ARG:HD2	2.01	0.41
1:A:291:ARG:HG3	1:A:292:ALA:N	2.35	0.41
1:A:418:ILE:HD12	1:A:447:LEU:HD21	2.02	0.41
1:A:267:ILE:HD11	1:A:448:TYR:CD2	2.56	0.41
1:A:364:ARG:HG3	1:A:364:ARG:NH1	2.34	0.41
1:A:439:SER:O	1:A:443:LYS:HA	2.20	0.41
1:A:259:LEU:HA	1:A:438:PRO:HB3	2.02	0.40
1:A:403:VAL:CG2	1:A:431:ARG:HH12	2.32	0.40
1:A:285:VAL:CG2	1:A:286:TYR:N	2.83	0.40

There are no symmetry-related clashes.

## 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	195/219 (89%)	161 (83%)	27 (14%)	7 (4%)	<b>3</b> <b>14</b>

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	301	GLU
1	A	370	LEU
1	A	378	THR
1	A	379	SER
1	A	410	VAL
1	A	453	ARG
1	A	377	ARG

### 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	171/190 (90%)	150 (88%)	21 (12%)	<b>4</b> <b>14</b>

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	HIS
1	A	261	LYS
1	A	263	THR
1	A	276	ARG
1	A	285	VAL
1	A	293	ARG
1	A	302	ASP
1	A	304	ASN
1	A	315	ARG
1	A	340	LEU
1	A	348	ARG
1	A	359	ASN
1	A	361	LEU
1	A	367	LYS
1	A	370	LEU
1	A	394	ARG
1	A	412	ASP
1	A	414	ASN
1	A	426	ARG
1	A	432	LEU

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Mol	Chain	Res	Type
1	A	437	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	258	HIS
1	A	288	GLN
1	A	304	ASN
1	A	332	ASN
1	A	359	ASN
1	A	376	HIS
1	A	414	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

1 ligand is 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	IPA	A	6001	-	3,3,3	0.43	0	3,3,3	0.41	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.

No monomer is involved in short contacts.

## 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 [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	197/219 (89%)	0.35	1 (0%) 91 91	49, 70, 102, 111	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	259	LEU	2.1

### 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 monosaccharides 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(Å <sup>2</sup> )	Q<0.9
2	IPA	A	6001	4/4	0.87	0.30	77,77,77,78	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.