



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:34 PM UTC

PDB ID : 1LBV / pdb_00001lbv
Title : Crystal Structure of apo-form (P21) of dual activity FBPase/IMPase (AF2372) from *Archaeoglobus fulgidus*
Authors : Stieglitz, K.A.; Johnson, K.A.; Yang, H.; Roberts, M.F.; Seaton, B.A.; Head, J.F.; Stec, B.
Deposited on : 2002-04-04
Resolution : 1.80 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

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>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

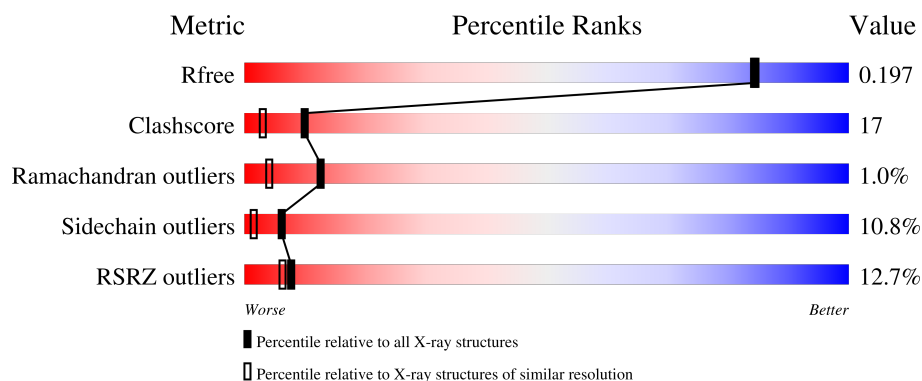
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 $\leq 5\%$. 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	252	4% 78% 19% .
1	B	252	21% 56% 34% 10% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4165 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 fructose 1,6-bisphosphatase/inositol monophosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			1966	1243	333	380	10			
1	B	252	Total	C	N	O	S	0	0	0
			1966	1243	333	380	10			

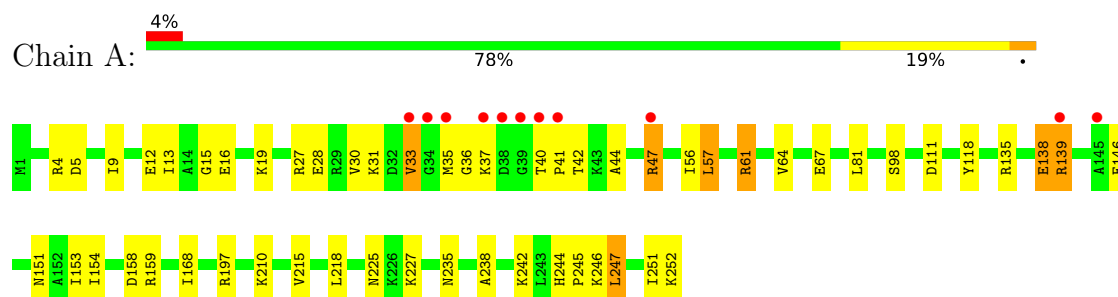
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	160	Total	O	0	0
			160	160		
2	B	73	Total	O	0	0
			73	73		

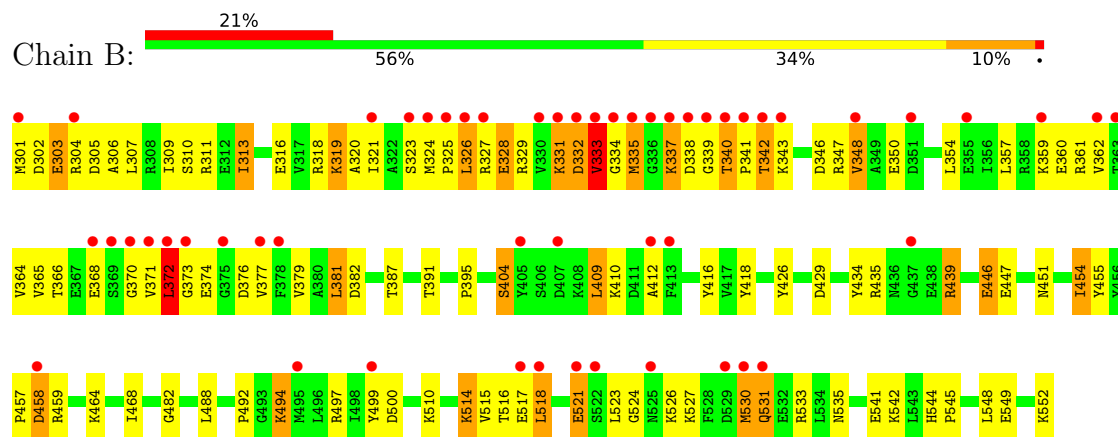
3 Residue-property plots

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: fructose 1,6-bisphosphatase/inositol monophosphatase



- Molecule 1: fructose 1,6-bisphosphatase/inositol monophosphatase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.81Å 53.25Å 82.15Å 90.00° 105.05° 90.00°	Depositor
Resolution (Å)	31.81 – 1.80 31.81 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.0 (31.81-1.80) 91.1 (31.81-1.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 1.79Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.203 , 0.273 0.200 , 0.197	Depositor DCC
R_{free} test set	3166 reflections (8.56%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4165	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.63% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.45	0/1999	1.28	8/2688 (0.3%)
1	B	0.39	0/1999	1.24	5/2688 (0.2%)
All	All	0.42	0/3998	1.26	13/5376 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	328	GLU	CA-C-N	7.19	130.25	120.54
1	B	328	GLU	C-N-CA	7.19	130.25	120.54
1	A	111	ASP	CA-CB-CG	-6.45	106.15	112.60
1	B	457	PRO	CA-C-N	6.22	132.16	122.26
1	B	457	PRO	C-N-CA	6.22	132.16	122.26
1	B	451	ASN	CA-CB-CG	-5.85	106.75	112.60
1	A	235	ASN	CA-CB-CG	5.72	118.32	112.60
1	A	4	ARG	CA-C-N	5.21	127.27	120.28
1	A	4	ARG	C-N-CA	5.21	127.27	120.28
1	A	153	ILE	CA-C-N	-5.08	114.20	122.33
1	A	153	ILE	C-N-CA	-5.08	114.20	122.33
1	A	247	LEU	CA-C-O	5.05	125.77	120.42
1	A	151	ASN	CA-CB-CG	-5.02	107.58	112.60

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	1966	0	1949	40	0
1	B	1966	0	1946	97	0
2	A	160	0	0	7	0
2	B	73	0	0	9	0
All	All	4165	0	3895	136	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 17.

All (136) 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:12:GLU:HG2	1:A:56:ILE:HD13	1.52	0.89
1:B:334:GLY:HA3	1:B:342:THR:HB	1.57	0.87
1:A:139:ARG:HB2	1:A:139:ARG:HH11	1.42	0.84
1:B:362:VAL:HG12	1:B:377:VAL:HB	1.62	0.81
1:A:168:ILE:HD12	1:B:468:ILE:HG13	1.67	0.76
1:A:35:MET:HA	1:A:41:PRO:HA	1.66	0.75
1:B:365:VAL:HG12	1:B:499:TYR:HE2	1.49	0.75
1:B:387:THR:O	1:B:391:THR:HG23	1.87	0.73
1:B:321:ILE:O	1:B:324:MET:HB2	1.89	0.72
1:A:158:ASP:OD1	1:A:159:ARG:HD3	1.91	0.70
1:B:307:LEU:O	1:B:311:ARG:HG3	1.92	0.69
1:B:320:ALA:HB1	1:B:348:VAL:HG13	1.74	0.69
1:A:16:GLU:HG2	2:A:1055:HOH:O	1.94	0.68
1:B:517:GLU:HG3	1:B:518:LEU:H	1.58	0.68
1:B:316:GLU:HA	1:B:319:LYS:HZ2	1.59	0.68
1:B:324:MET:HE3	1:B:348:VAL:HG21	1.77	0.67
1:B:316:GLU:HA	1:B:319:LYS:NZ	2.10	0.66
1:B:332:ASP:HB2	1:B:341:PRO:HB2	1.78	0.66
1:B:332:ASP:O	1:B:333:VAL:HG13	1.97	0.64
1:B:305:ASP:O	1:B:309:ILE:HG13	1.97	0.64
1:B:410:LYS:HD3	1:B:524:GLY:HA3	1.80	0.63
1:A:246:LYS:HD3	2:A:1205:HOH:O	1.99	0.63
1:B:492:PRO:HA	2:B:1071:HOH:O	1.99	0.62
1:B:332:ASP:HA	1:B:343:LYS:HA	1.80	0.62
1:A:35:MET:HE3	1:A:41:PRO:HD3	1.82	0.62
1:A:15:GLY:O	1:A:19:LYS:HG3	2.01	0.61
1:B:339:GLY:O	1:B:340:THR:HG23	2.01	0.61
1:A:67:GLU:HG3	1:A:197:ARG:NH2	2.16	0.60
1:A:28:GLU:OE2	1:A:31:LYS:HE3	2.01	0.60
1:B:454:ILE:HD13	1:B:488:LEU:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:ASP:HB3	1:B:459:ARG:HD3	1.84	0.60
1:B:309:ILE:O	1:B:313:ILE:HD12	2.02	0.59
1:B:365:VAL:HG12	1:B:499:TYR:CE2	2.35	0.59
1:B:350:GLU:HG2	1:B:354:LEU:HD11	1.83	0.58
1:B:318:ARG:HD2	1:B:418:TYR:HE2	1.68	0.58
1:B:301:MET:HG3	1:B:305:ASP:HB2	1.85	0.58
1:A:225:ASN:HB2	2:A:1096:HOH:O	2.02	0.58
1:A:98:SER:HB3	1:A:118:TYR:O	2.04	0.58
1:B:497:ARG:HD3	2:B:1145:HOH:O	2.05	0.56
1:B:371:VAL:O	1:B:372:LEU:HB2	2.05	0.56
1:B:545:PRO:O	1:B:549:GLU:HG3	2.07	0.54
1:B:446:GLU:OE2	1:B:542:LYS:HD3	2.08	0.54
1:B:545:PRO:HA	1:B:548:LEU:HD12	1.89	0.54
1:B:361:ARG:H	1:B:361:ARG:HD2	1.73	0.54
1:B:362:VAL:HG12	1:B:377:VAL:CB	2.36	0.54
1:B:372:LEU:HD23	1:B:373:GLY:N	2.23	0.53
1:B:332:ASP:CB	1:B:341:PRO:HB2	2.40	0.53
1:B:301:MET:HG3	1:B:305:ASP:CB	2.39	0.52
1:A:247:LEU:O	1:A:251:ILE:HG12	2.09	0.52
1:B:350:GLU:HG2	1:B:354:LEU:CD1	2.40	0.52
1:B:366:THR:CG2	1:B:381:LEU:HD23	2.40	0.52
1:B:323:SER:O	1:B:325:PRO:HD3	2.10	0.51
1:B:434:TYR:CE2	1:B:439:ARG:HG3	2.46	0.51
1:B:357:LEU:HD13	1:B:364:VAL:HG22	1.93	0.51
1:B:429:ASP:O	1:B:510:LYS:HD2	2.10	0.51
1:A:28:GLU:CD	1:A:31:LYS:HE3	2.36	0.51
1:A:12:GLU:HG2	1:A:56:ILE:CD1	2.35	0.50
1:A:146:GLU:OE1	1:A:242:LYS:HD2	2.12	0.50
1:B:361:ARG:HD2	1:B:361:ARG:N	2.27	0.50
1:B:366:THR:HG22	1:B:381:LEU:HD23	1.93	0.50
1:B:382:ASP:OD2	1:B:500:ASP:OD2	2.30	0.50
1:B:497:ARG:HH22	1:B:530:MET:HE3	1.77	0.50
1:B:338:ASP:O	1:B:338:ASP:OD1	2.30	0.49
1:B:517:GLU:OE2	1:B:526:LYS:HE3	2.11	0.49
1:B:530:MET:O	1:B:530:MET:HG3	2.13	0.49
1:A:139:ARG:HH11	1:A:139:ARG:CB	2.20	0.49
1:A:30:VAL:O	1:A:30:VAL:HG22	2.12	0.48
1:B:329:ARG:HB3	1:B:391:THR:HG22	1.94	0.48
1:B:372:LEU:HD23	1:B:373:GLY:H	1.77	0.48
1:B:302:ASP:OD2	1:B:304:ARG:HB2	2.13	0.48
1:A:47:ARG:HE	1:A:47:ARG:HB3	1.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:LEU:HD12	1:A:81:LEU:HD22	1.96	0.48
1:B:429:ASP:O	1:B:510:LYS:HE3	2.12	0.48
1:B:379:VAL:HG12	1:B:379:VAL:O	2.14	0.48
1:B:318:ARG:HD2	1:B:418:TYR:CE2	2.49	0.47
1:B:327:ARG:HH11	1:B:327:ARG:HG2	1.79	0.47
1:B:331:LYS:O	1:B:343:LYS:HA	2.13	0.47
1:B:410:LYS:CD	1:B:524:GLY:HA3	2.44	0.47
1:B:404:SER:HA	1:B:412:ALA:HA	1.95	0.47
1:B:516:THR:C	1:B:523:LEU:HD21	2.39	0.47
1:B:516:THR:HB	1:B:521:GLU:O	2.15	0.47
1:B:334:GLY:HA3	1:B:342:THR:CB	2.38	0.46
1:B:357:LEU:HD13	1:B:364:VAL:CG2	2.46	0.46
1:B:303:GLU:CD	1:B:429:ASP:HB2	2.41	0.46
1:A:13:ILE:HA	1:A:56:ILE:HD12	1.98	0.46
1:B:517:GLU:HG3	1:B:518:LEU:N	2.28	0.46
1:B:365:VAL:HG13	1:B:370:GLY:O	2.15	0.46
1:B:458:ASP:CB	1:B:459:ARG:HH11	2.29	0.46
1:B:464:LYS:NZ	2:B:1189:HOH:O	2.49	0.45
1:A:35:MET:HG2	1:A:36:GLY:O	2.16	0.45
1:B:359:LYS:HG2	1:B:359:LYS:O	2.16	0.45
1:B:435:ARG:NH1	2:B:1193:HOH:O	2.50	0.45
1:A:33:VAL:HG21	1:A:44:ALA:HA	1.99	0.45
1:B:365:VAL:HA	1:B:370:GLY:O	2.17	0.45
1:B:514:LYS:HD3	1:B:544:HIS:CG	2.52	0.45
1:A:13:ILE:HD11	1:A:57:LEU:HG	1.98	0.45
1:B:303:GLU:O	1:B:306:ALA:N	2.50	0.44
1:A:61:ARG:NH1	2:A:1058:HOH:O	2.50	0.44
1:A:227:LYS:HD2	2:A:1167:HOH:O	2.17	0.44
1:A:244:HIS:N	1:A:245:PRO:HD2	2.33	0.44
1:B:302:ASP:O	1:B:305:ASP:HB2	2.17	0.44
1:B:319:LYS:NZ	2:B:1198:HOH:O	2.50	0.44
1:B:301:MET:N	2:B:1099:HOH:O	2.50	0.44
1:A:135:ARG:O	1:A:138:GLU:HG3	2.18	0.44
1:A:57:LEU:HD13	1:A:64:VAL:HG22	2.00	0.43
1:B:531:GLN:OE1	1:B:533:ARG:NH2	2.50	0.43
1:B:346:ASP:OD1	1:B:387:THR:OG1	2.30	0.43
1:B:458:ASP:HB2	1:B:459:ARG:HH11	1.83	0.43
1:B:362:VAL:HG12	1:B:377:VAL:CG1	2.49	0.43
1:B:499:TYR:OH	1:B:530:MET:HA	2.19	0.43
1:A:5:ASP:O	1:A:9:ILE:HD12	2.18	0.42
1:B:482:GLY:HA2	2:B:1113:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:ALA:HB1	1:B:348:VAL:CG1	2.44	0.42
1:B:337:LYS:HE3	1:B:531:GLN:HE22	1.84	0.42
1:A:33:VAL:HB	1:A:47:ARG:HD3	2.01	0.42
1:A:35:MET:HE2	1:A:40:THR:HA	2.01	0.42
1:B:426:TYR:CZ	1:B:435:ARG:HD2	2.55	0.41
1:A:159:ARG:HD2	2:A:1078:HOH:O	2.20	0.41
1:B:395:PRO:HD3	2:B:1124:HOH:O	2.20	0.41
1:B:326:LEU:HD23	1:B:326:LEU:HA	1.79	0.41
1:A:19:LYS:HB3	1:A:19:LYS:HE3	1.86	0.41
1:A:56:ILE:HD13	1:A:56:ILE:HG21	1.82	0.41
1:B:310:SER:HB3	1:B:416:TYR:CD2	2.55	0.41
1:A:42:THR:HG21	1:A:47:ARG:HD2	2.01	0.41
1:B:494:LYS:HG3	1:B:535:ASN:OD1	2.20	0.41
1:B:316:GLU:OE1	1:B:319:LYS:NZ	2.50	0.41
1:B:409:LEU:HD22	1:B:409:LEU:HA	1.92	0.41
1:B:497:ARG:NH2	1:B:530:MET:HE3	2.35	0.41
1:B:454:ILE:HD12	1:B:455:TYR:N	2.36	0.41
1:B:447:GLU:OE1	1:B:447:GLU:HA	2.21	0.40
1:B:521:GLU:HB2	2:B:1196:HOH:O	2.20	0.40
1:A:210:LYS:HG2	2:A:1012:HOH:O	2.20	0.40
1:A:159:ARG:HH22	1:A:251:ILE:C	2.29	0.40
1:A:215:VAL:HG22	1:A:238:ALA:CB	2.51	0.40
1:B:518:LEU:HD12	1:B:518:LEU:HA	1.71	0.40
1:B:515:VAL:HG12	1:B:523:LEU:HD11	2.02	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	250/252 (99%)	237 (95%)	13 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	250/252 (99%)	228 (91%)	17 (7%)	5 (2%)	6	1
All	All	500/504 (99%)	465 (93%)	30 (6%)	5 (1%)	12	4

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	333	VAL
1	B	335	MET
1	B	342	THR
1	B	368	GLU
1	B	372	LEU

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	204/204 (100%)	193 (95%)	11 (5%)	20	8
1	B	204/204 (100%)	171 (84%)	33 (16%)	2	0
All	All	408/408 (100%)	364 (89%)	44 (11%)	6	1

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ARG
1	A	33	VAL
1	A	37	LYS
1	A	47	ARG
1	A	57	LEU
1	A	61	ARG
1	A	138	GLU
1	A	139	ARG
1	A	154	ILE
1	A	218	LEU
1	A	252	LYS

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Mol	Chain	Res	Type
1	B	303	GLU
1	B	313	ILE
1	B	319	LYS
1	B	326	LEU
1	B	328	GLU
1	B	331	LYS
1	B	332	ASP
1	B	333	VAL
1	B	335	MET
1	B	337	LYS
1	B	340	THR
1	B	347	ARG
1	B	348	VAL
1	B	360	GLU
1	B	372	LEU
1	B	374	GLU
1	B	376	ASP
1	B	381	LEU
1	B	404	SER
1	B	409	LEU
1	B	439	ARG
1	B	446	GLU
1	B	454	ILE
1	B	458	ASP
1	B	494	LYS
1	B	514	LYS
1	B	518	LEU
1	B	521	GLU
1	B	527	LYS
1	B	530	MET
1	B	531	GLN
1	B	541	GLU
1	B	552	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	235	ASN
1	B	525	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 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	252/252 (100%)	0.20	11 (4%)	39 38	12, 20, 44, 72	0
1	B	252/252 (100%)	1.20	53 (21%)	2 2	16, 34, 79, 141	0
All	All	504/504 (100%)	0.70	64 (12%)	8 6	12, 26, 64, 141	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	341	PRO	6.2
1	B	342	THR	5.7
1	B	334	GLY	5.7
1	B	340	THR	5.1
1	B	333	VAL	4.9
1	B	337	LYS	4.8
1	B	372	LEU	4.7
1	B	338	ASP	4.6
1	B	370	GLY	4.5
1	B	304	ARG	4.0
1	B	330	VAL	4.0
1	B	339	GLY	4.0
1	A	34	GLY	3.9
1	A	145	ALA	3.6
1	A	33	VAL	3.6
1	B	335	MET	3.6
1	A	40	THR	3.5
1	B	321	ILE	3.4
1	B	373	GLY	3.3
1	B	375	GLY	3.3
1	B	327	ARG	3.3
1	B	325	PRO	3.3
1	A	38	ASP	3.3
1	B	405	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	371	VAL	3.2
1	B	407	ASP	3.2
1	B	531	GLN	3.1
1	B	518	LEU	3.0
1	A	39	GLY	3.0
1	B	362	VAL	3.0
1	B	363	THR	2.9
1	B	324	MET	2.9
1	A	41	PRO	2.9
1	B	359	LYS	2.8
1	B	530	MET	2.8
1	B	377	VAL	2.8
1	A	47	ARG	2.7
1	B	368	GLU	2.7
1	B	348	VAL	2.7
1	B	323	SER	2.7
1	A	37	LYS	2.7
1	B	331	LYS	2.7
1	B	336	GLY	2.6
1	B	301	MET	2.5
1	B	529	ASP	2.5
1	A	35	MET	2.5
1	B	412	ALA	2.5
1	B	495	MET	2.4
1	B	525	ASN	2.4
1	B	326	LEU	2.4
1	A	139	ARG	2.3
1	B	369	SER	2.3
1	B	521	GLU	2.3
1	B	343	LYS	2.2
1	B	351	ASP	2.1
1	B	355	GLU	2.1
1	B	437	GLY	2.1
1	B	517	GLU	2.1
1	B	332	ASP	2.1
1	B	458	ASP	2.1
1	B	499	TYR	2.1
1	B	522	SER	2.1
1	B	378	PHE	2.0
1	B	413	PHE	2.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.