



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:39 PM GMT

PDB ID : 1LBW
Title : Crystal Structure of apo-form (P32) 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 : 2.00 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
<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

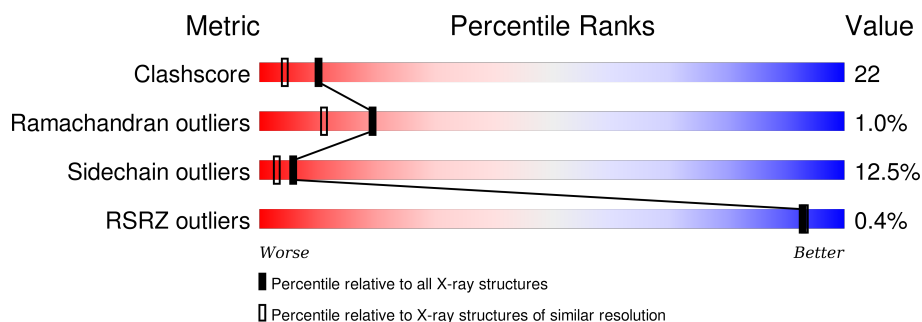
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	252	
1	B	252	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4068 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			

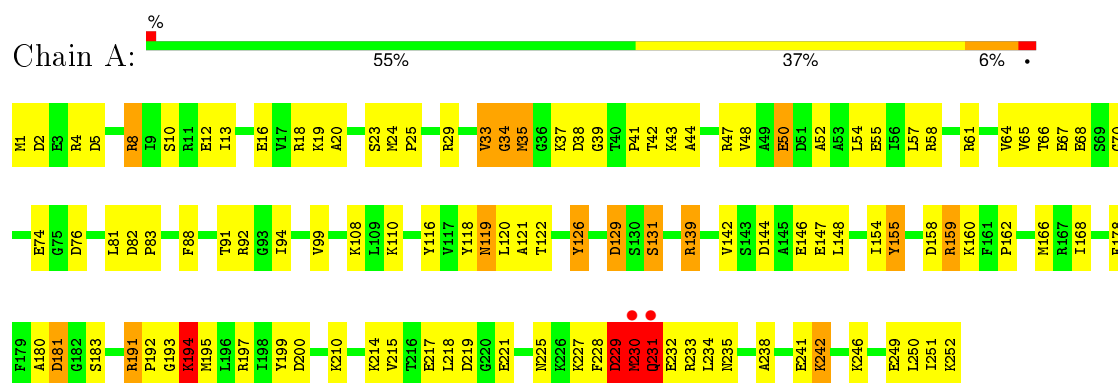
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	70	Total	O	0	0
			70	70		
2	B	66	Total	O	0	0
			66	66		

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: 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 32	Depositor
Cell constants a, b, c, α , β , γ	89.37Å 89.37Å 103.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.00 38.70 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (30.00-2.00) 92.7 (38.70-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.77 (at 2.00Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.186 , 0.203 0.173 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.0	EDS
Estimated twinning fraction	0.027 for -h,-k,l 0.487 for h,-h-k,-l 0.027 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 57501 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4068	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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

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	1.27	12/2688 (0.4%)
1	B	0.39	0/1999	1.20	8/2688 (0.3%)
All	All	0.42	0/3998	1.24	20/5376 (0.4%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	435	ARG	CD-NE-CZ	15.60	145.44	123.60
1	A	33	VAL	C-N-CA	11.11	145.62	122.30
1	A	18	ARG	CD-NE-CZ	9.88	137.43	123.60
1	A	139	ARG	NE-CZ-NH1	-8.88	115.86	120.30
1	A	18	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	B	304	ARG	NE-CZ-NH1	-6.55	117.03	120.30
1	B	467	ARG	NE-CZ-NH1	-6.42	117.09	120.30
1	A	129	ASP	CB-CG-OD1	6.24	123.91	118.30
1	B	347	ARG	CD-NE-CZ	6.18	132.25	123.60
1	A	58	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	A	180	ALA	C-N-CA	5.88	136.39	121.70
1	A	230	MET	C-N-CA	5.85	136.32	121.70
1	A	61	ARG	CD-NE-CZ	5.83	131.77	123.60
1	A	191	ARG	NE-CZ-NH1	-5.81	117.40	120.30
1	A	155	TYR	C-N-CA	5.27	134.88	121.70
1	B	435	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	2	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	499	TYR	CB-CG-CD1	-5.12	117.93	121.00
1	B	439	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	B	499	TYR	CB-CG-CD2	5.09	124.06	121.00

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	1948	92	0
1	B	1966	0	1946	83	0
2	A	70	0	0	3	0
2	B	66	0	0	3	0
All	All	4068	0	3894	171	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 22.

All (171) 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:B:342:THR:HG21	1:B:347:ARG:HE	1.26	1.01
1:A:119:ASN:HD22	1:A:121:ALA:H	1.25	0.84
1:B:432:GLY:HA3	1:B:439:ARG:HH21	1.47	0.79
1:A:108:LYS:HD3	1:A:225:ASN:HA	1.68	0.76
1:B:408:LYS:HG2	1:B:527:LYS:HD3	1.66	0.76
1:B:337:LYS:HD2	1:B:370:GLY:HA3	1.68	0.74
1:A:65:VAL:HG11	1:A:228:PHE:O	1.88	0.74
1:A:194:LYS:HG2	1:A:235:ASN:ND2	2.04	0.73
1:B:451:ASN:HD22	1:B:465:ARG:HB2	1.55	0.72
1:A:148:LEU:HD22	1:A:250:LEU:HD22	1.73	0.71
1:B:535:ASN:O	1:B:536:ILE:HD13	1.90	0.70
1:A:44:ALA:O	1:A:48:VAL:HG23	1.91	0.69
1:A:34:GLY:O	1:A:41:PRO:HA	1.92	0.69
1:A:119:ASN:ND2	1:A:121:ALA:H	1.92	0.68
1:A:197:ARG:HD3	1:A:199:TYR:OH	1.93	0.67
1:A:34:GLY:HA2	1:A:42:THR:O	1.94	0.67
1:B:432:GLY:HA3	1:B:439:ARG:NH2	2.10	0.66
1:B:342:THR:HG21	1:B:347:ARG:NE	2.07	0.65
1:B:318:ARG:HG3	2:B:1019:HOH:O	1.96	0.65
1:B:365:VAL:HG21	1:B:528:PHE:O	1.96	0.65
1:A:193:GLY:O	1:A:195:MET:HG2	1.97	0.64
1:A:33:VAL:HG11	2:A:1101:HOH:O	1.98	0.64
1:A:219:ASP:OD1	1:A:221:GLU:HG3	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:ASP:O	1:B:510:LYS:HD2	1.98	0.64
1:B:367:GLU:HG3	1:B:499:TYR:CE1	2.33	0.64
1:A:158:ASP:O	1:B:459:ARG:HA	1.98	0.63
1:A:146:GLU:HG3	1:A:242:LYS:HB3	1.81	0.62
1:B:505:VAL:HG13	1:B:515:VAL:HG11	1.82	0.61
1:A:47:ARG:HA	1:A:68:GLU:OE1	1.99	0.61
1:A:168:ILE:HD12	1:B:468:ILE:HG13	1.81	0.61
1:A:118:TYR:HD2	1:A:120:LEU:HD23	1.67	0.60
1:B:494:LYS:HE2	1:B:535:ASN:OD1	2.02	0.60
1:A:119:ASN:HD21	1:A:121:ALA:HB3	1.67	0.60
1:A:195:MET:O	1:A:233:ARG:HD2	2.01	0.60
1:A:146:GLU:O	1:A:146:GLU:HG2	2.01	0.59
1:B:399:VAL:HG22	1:B:420:LEU:HD11	1.83	0.59
1:A:119:ASN:HD22	1:A:121:ALA:N	1.98	0.59
1:A:1:MET:HG3	1:A:5:ASP:HB2	1.85	0.59
1:B:534:LEU:HD12	1:B:536:ILE:HD11	1.85	0.58
1:A:146:GLU:HG2	1:A:246:LYS:NZ	2.19	0.58
1:A:146:GLU:HG2	1:A:246:LYS:HZ2	1.68	0.58
1:A:67:GLU:HG3	1:A:199:TYR:OH	2.03	0.57
1:A:146:GLU:OE1	1:A:242:LYS:HD3	2.04	0.57
1:B:361:ARG:CZ	1:B:375:GLY:HA2	2.34	0.57
1:A:158:ASP:OD1	1:A:159:ARG:HD3	2.05	0.57
1:B:361:ARG:O	1:B:361:ARG:HG3	2.03	0.57
1:B:369:SER:OG	1:B:372:LEU:HD11	2.07	0.55
1:A:217:GLU:OE1	1:A:235:ASN:HB2	2.07	0.55
1:B:407:ASP:HB3	1:B:527:LYS:NZ	2.22	0.54
1:B:451:ASN:ND2	1:B:465:ARG:HB2	2.22	0.54
1:A:129:ASP:OD1	1:A:131:SER:HB3	2.08	0.54
1:A:230:MET:O	1:A:232:GLU:N	2.41	0.54
1:A:67:GLU:OE1	1:A:197:ARG:NE	2.41	0.54
1:A:92:ARG:HG2	1:B:483:SER:HB2	1.90	0.54
1:A:38:ASP:HB2	1:A:67:GLU:OE2	2.09	0.53
1:B:546:LYS:O	1:B:549:GLU:HB3	2.08	0.53
1:A:118:TYR:CD2	1:A:120:LEU:HD23	2.43	0.53
1:B:407:ASP:OD1	1:B:527:LYS:NZ	2.41	0.53
1:A:37:LYS:HG3	1:A:70:GLY:CA	2.39	0.53
1:A:66:THR:HG22	1:A:81:LEU:O	2.09	0.52
1:B:354:LEU:O	1:B:358:ARG:HB2	2.09	0.52
1:A:50:GLU:OE2	1:A:83:PRO:HG3	2.10	0.51
1:B:407:ASP:HB3	1:B:527:LYS:HZ3	1.75	0.51
1:B:366:THR:O	1:B:370:GLY:HA2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ARG:HG3	1:A:233:ARG:HD3	1.92	0.50
1:A:219:ASP:OD2	1:A:221:GLU:OE1	2.30	0.50
1:B:338:ASP:OD1	1:B:340:THR:OG1	2.29	0.50
1:B:327:ARG:HG3	1:B:328:GLU:N	2.25	0.50
1:B:428:ALA:HB1	1:B:510:LYS:HG3	1.93	0.50
1:B:445:ALA:HB2	1:B:485:ASP:OD1	2.11	0.50
1:B:450:CYS:HB2	1:B:485:ASP:OD2	2.12	0.50
1:A:82:ASP:OD2	1:A:200:ASP:OD1	2.29	0.50
1:B:382:ASP:OD2	1:B:500:ASP:OD1	2.30	0.50
1:A:20:ALA:HB1	1:A:48:VAL:HG12	1.94	0.49
1:A:119:ASN:ND2	1:A:121:ALA:HB3	2.26	0.49
1:A:214:LYS:HD2	1:A:241:GLU:OE2	2.12	0.49
1:A:65:VAL:HG21	1:A:228:PHE:HB3	1.95	0.49
1:B:501:ALA:O	1:B:505:VAL:HG23	2.13	0.49
1:B:312:GLU:OE2	1:B:356:ILE:HD12	2.12	0.49
1:A:228:PHE:O	1:A:229:ASP:O	2.29	0.49
1:A:37:LYS:HB2	1:A:67:GLU:O	2.12	0.49
1:A:12:GLU:HG2	2:A:1065:HOH:O	2.11	0.49
1:A:197:ARG:HD3	1:A:199:TYR:CZ	2.48	0.49
1:B:371:VAL:O	1:B:372:LEU:HD23	2.12	0.49
1:B:325:PRO:HG2	1:B:328:GLU:HG2	1.94	0.49
1:B:435:ARG:HB2	1:B:440:ILE:HG21	1.94	0.49
1:B:318:ARG:HA	1:B:420:LEU:HD22	1.95	0.48
1:A:8:ARG:O	1:A:12:GLU:HG3	2.13	0.48
1:A:249:GLU:O	1:A:252:LYS:HB2	2.14	0.48
1:A:230:MET:CG	1:A:231:GLN:H	2.25	0.48
1:B:388:PHE:O	1:B:392:ARG:HG2	2.14	0.48
1:A:215:VAL:HG13	1:A:238:ALA:HB2	1.95	0.48
1:B:330:VAL:HG22	1:B:330:VAL:O	2.13	0.48
1:B:410:LYS:HB3	1:B:524:GLY:O	2.14	0.47
1:A:20:ALA:HB1	1:A:48:VAL:CG1	2.45	0.47
1:B:467:ARG:HG3	1:B:484:PHE:CZ	2.50	0.47
1:A:154:ILE:HG21	1:A:166:MET:HG2	1.96	0.47
1:B:351:ASP:O	1:B:355:GLU:HG2	2.15	0.47
1:A:194:LYS:O	1:A:233:ARG:HB2	2.15	0.47
1:B:465:ARG:HG3	1:B:465:ARG:HH11	1.80	0.47
1:B:494:LYS:O	1:B:533:ARG:HD2	2.14	0.47
1:A:50:GLU:OE1	1:A:68:GLU:HB3	2.14	0.47
1:A:155:TYR:O	1:A:191:ARG:HG3	2.15	0.47
1:A:67:GLU:HB2	1:A:199:TYR:CZ	2.50	0.46
1:B:544:HIS:N	1:B:545:PRO:HD2	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:LYS:HE2	1:B:527:LYS:HD3	1.96	0.46
1:A:194:LYS:HG2	1:A:235:ASN:HD21	1.79	0.46
1:B:338:ASP:OD2	1:B:367:GLU:HG2	2.15	0.46
1:A:119:ASN:ND2	1:A:122:THR:H	2.13	0.46
1:A:126:TYR:HE2	1:A:181:ASP:OD1	1.99	0.46
1:B:307:LEU:HD13	1:B:414:PHE:HZ	1.81	0.45
1:B:337:LYS:CD	1:B:370:GLY:HA3	2.44	0.45
1:A:10:SER:HB3	1:A:116:TYR:CD2	2.52	0.45
1:B:350:GLU:O	1:B:354:LEU:HG	2.16	0.45
1:A:91:THR:OG1	1:A:92:ARG:NH1	2.50	0.45
1:B:544:HIS:CE1	1:B:548:LEU:HD11	2.51	0.45
1:B:340:THR:HB	1:B:341:PRO:HD2	1.98	0.45
1:A:16:GLU:HB3	1:A:52:ALA:HB1	1.98	0.45
1:A:210:LYS:HD3	1:A:210:LYS:HA	1.76	0.45
1:B:438:GLU:HG3	1:B:439:ARG:O	2.18	0.44
1:A:29:ARG:O	1:A:43:LYS:HB3	2.17	0.44
1:A:233:ARG:C	1:A:234:LEU:HD23	2.38	0.44
1:B:495:MET:N	2:B:1011:HOH:O	2.50	0.44
1:B:517:GLU:HG2	1:B:523:LEU:HD21	1.99	0.44
1:B:416:TYR:CE2	1:B:418:TYR:HB2	2.53	0.44
1:B:338:ASP:HB3	1:B:367:GLU:HG2	2.00	0.44
1:B:318:ARG:O	1:B:318:ARG:HG2	2.17	0.44
1:B:338:ASP:CB	1:B:367:GLU:HG2	2.48	0.44
1:B:467:ARG:HG3	1:B:484:PHE:HZ	1.83	0.44
1:A:99:VAL:HG12	1:A:120:LEU:HD21	1.99	0.44
1:B:363:THR:O	1:B:378:PHE:HA	2.17	0.44
1:A:66:THR:CG2	1:A:81:LEU:HD23	2.49	0.43
1:A:234:LEU:N	1:A:234:LEU:HD23	2.33	0.43
1:A:146:GLU:CD	1:A:242:LYS:HD3	2.38	0.43
1:B:443:SER:OG	1:B:445:ALA:HB2	2.18	0.43
1:B:419:ASN:OD1	1:B:422:THR:HG23	2.18	0.43
1:A:13:ILE:HD11	1:A:57:LEU:HG	1.99	0.43
1:A:24:MET:HA	1:A:25:PRO:HD3	1.74	0.43
1:B:314:ALA:HB1	1:B:418:TYR:CD2	2.54	0.43
1:A:10:SER:HB3	1:A:116:TYR:CG	2.53	0.43
1:B:531:GLN:HB2	2:B:1104:HOH:O	2.18	0.43
1:B:385:ASP:O	1:B:397:TYR:HA	2.19	0.43
1:A:191:ARG:HA	1:A:192:PRO:HD3	1.85	0.43
1:A:67:GLU:CG	1:A:199:TYR:OH	2.67	0.43
1:A:37:LYS:HG2	1:A:67:GLU:O	2.19	0.43
1:B:410:LYS:N	1:B:524:GLY:O	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:PHE:O	1:A:92:ARG:HD2	2.19	0.42
1:B:426:TYR:CE1	1:B:435:ARG:HG3	2.54	0.42
1:A:232:GLU:HA	1:A:232:GLU:OE2	2.19	0.42
1:B:521:GLU:HG3	1:B:522:SER:N	2.33	0.42
1:B:465:ARG:HG3	1:B:465:ARG:NH1	2.34	0.42
1:A:54:LEU:HD21	1:A:64:VAL:HG11	2.02	0.42
1:B:449:TYR:CE1	1:B:464:LYS:HA	2.54	0.42
1:B:494:LYS:NZ	1:B:517:GLU:OE2	2.52	0.42
1:A:218:LEU:HA	1:A:218:LEU:HD12	1.89	0.42
1:A:148:LEU:HB3	1:A:162:PRO:HG2	2.00	0.41
1:B:491:ARG:HA	1:B:492:PRO:HD3	1.94	0.41
1:A:178:PHE:O	1:A:181:ASP:HB2	2.20	0.41
1:A:142:VAL:HG13	2:A:1004:HOH:O	2.20	0.41
1:B:447:GLU:OE1	1:B:447:GLU:HA	2.21	0.41
1:A:158:ASP:N	1:A:158:ASP:OD1	2.53	0.41
1:A:24:MET:CE	1:A:29:ARG:HA	2.51	0.41
1:A:35:MET:SD	1:A:39:GLY:HA2	2.61	0.41
1:B:514:LYS:O	1:B:538:ALA:HA	2.21	0.41
1:A:108:LYS:HB3	1:A:110:LYS:HG2	2.03	0.41
1:A:66:THR:HG21	1:A:81:LEU:HD23	2.04	0.41
1:B:359:LYS:HB2	1:B:359:LYS:HE2	1.83	0.40
1:B:451:ASN:HD21	1:B:465:ARG:HH11	1.69	0.40
1:A:181:ASP:HB3	1:A:183:SER:H	1.85	0.40
1:A:94:ILE:HG12	1:B:478:PHE:CZ	2.56	0.40
1:B:321:ILE:HD11	1:B:349:ALA:HB2	2.03	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%)	234 (94%)	12 (5%)	4 (2%)	12 5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	250/252 (99%)	239 (96%)	10 (4%)	1 (0%)	39	33
All	All	500/504 (99%)	473 (95%)	22 (4%)	5 (1%)	19	11

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229	ASP
1	A	231	GLN
1	A	194	LYS
1	B	445	ALA
1	A	34	GLY

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%)	179 (88%)	25 (12%)	6	3
1	B	204/204 (100%)	178 (87%)	26 (13%)	5	3
All	All	408/408 (100%)	357 (88%)	51 (12%)	6	3

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	8	ARG
1	A	19	LYS
1	A	23	SER
1	A	35	MET
1	A	50	GLU
1	A	55	GLU
1	A	74	GLU
1	A	76	ASP
1	A	119	ASN
1	A	126	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	131	SER
1	A	139	ARG
1	A	144	ASP
1	A	147	GLU
1	A	159	ARG
1	A	160	LYS
1	A	181	ASP
1	A	194	LYS
1	A	227	LYS
1	A	229	ASP
1	A	230	MET
1	A	231	GLN
1	A	242	LYS
1	A	251	ILE
1	B	302	ASP
1	B	303	GLU
1	B	318	ARG
1	B	347	ARG
1	B	359	LYS
1	B	360	GLU
1	B	361	ARG
1	B	366	THR
1	B	369	SER
1	B	399	VAL
1	B	403	PHE
1	B	406	SER
1	B	410	LYS
1	B	438	GLU
1	B	439	ARG
1	B	441	GLU
1	B	447	GLU
1	B	454	ILE
1	B	495	MET
1	B	498	ILE
1	B	499	TYR
1	B	517	GLU
1	B	519	ASP
1	B	533	ARG
1	B	534	LEU
1	B	552	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	231	GLN
1	A	235	ASN
1	B	389	ASN
1	B	451	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](#)

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 [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	252/252 (100%)	-0.66	2 (0%) 87 88	21, 36, 61, 120	0
1	B	252/252 (100%)	-0.66	0 100 100	23, 37, 58, 79	0
All	All	504/504 (100%)	-0.66	2 (0%) 93 93	21, 36, 60, 120	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	231	GLN	4.4
1	A	230	MET	2.6

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.