



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:26 PM UTC

PDB ID : 1LBW / pdb_00001lbw
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

<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

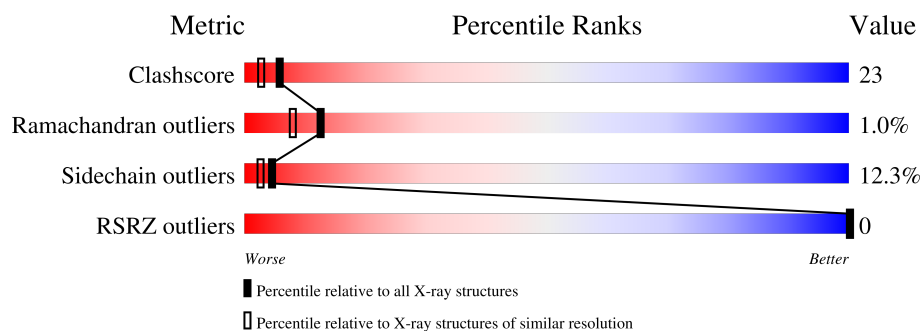
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 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	50% 43% 6% .
1	B	252	53% 37% 9% .

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			

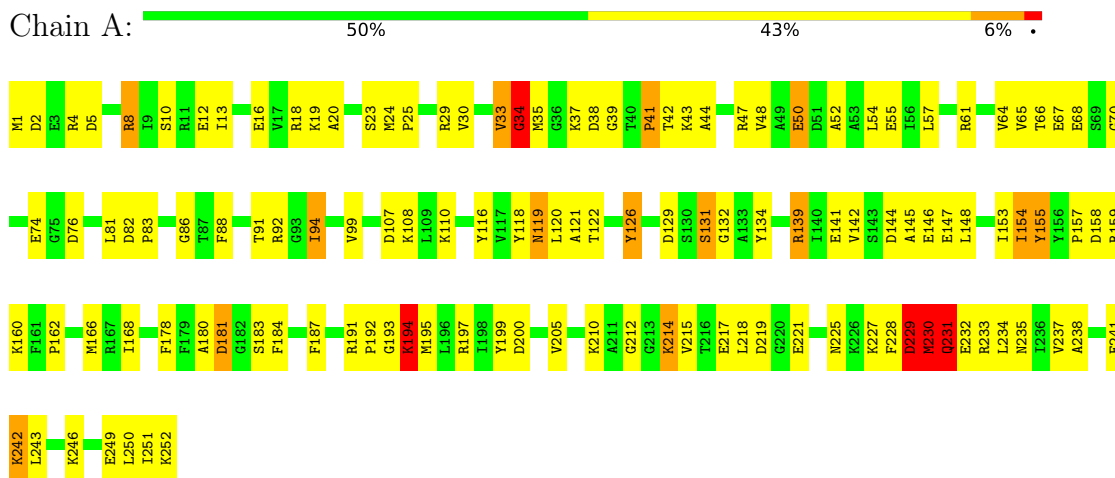
- Molecule 2 is water.

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

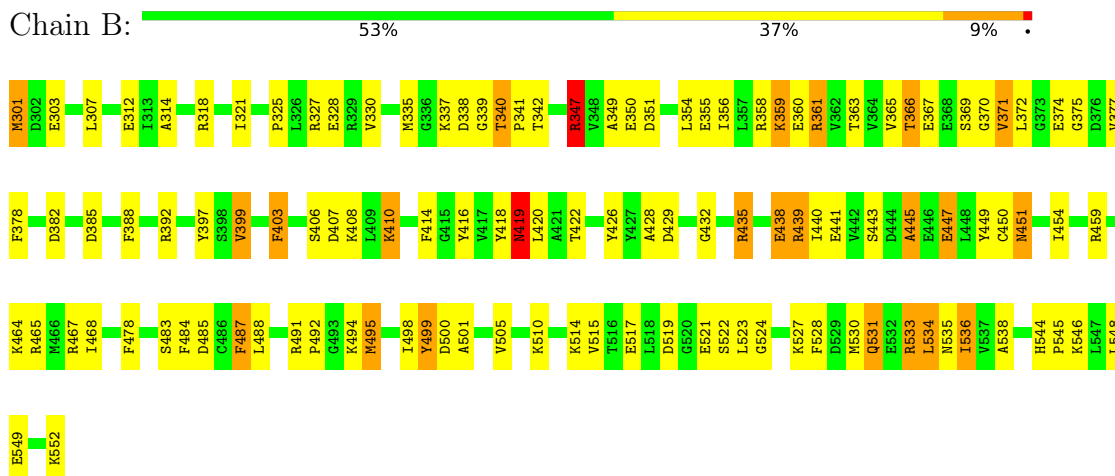
3 Residue-property plots

These plots are drawn for all protein, RNA, 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 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 30.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (30.00-2.00) 92.7 (30.00-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 2.00Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.186 , 0.203 0.172 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l 0.487 for h,-h-k,-l 0.026 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	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 5.55% 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	0.55	0/1999	1.72	46/2688 (1.7%)
1	B	0.46	0/1999	1.58	10/2688 (0.4%)
All	All	0.51	0/3998	1.65	56/5376 (1.0%)

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	435	ARG	CD-NE-CZ	15.03	145.44	124.40
1	A	33	VAL	CA-C-N	13.29	145.62	121.70
1	A	33	VAL	C-N-CA	13.29	145.62	121.70
1	A	180	ALA	CA-C-N	10.58	136.39	120.31
1	A	180	ALA	C-N-CA	10.58	136.39	120.31
1	A	229	ASP	CA-CB-CG	10.41	123.01	112.60
1	A	18	ARG	CD-NE-CZ	9.30	137.43	124.40
1	A	237	VAL	O-C-N	8.06	130.53	122.71
1	A	230	MET	CA-C-N	7.74	136.32	121.54
1	A	230	MET	C-N-CA	7.74	136.32	121.54
1	A	157	PRO	CA-C-N	7.39	133.38	122.08
1	A	157	PRO	C-N-CA	7.39	133.38	122.08
1	A	155	TYR	CA-C-N	7.32	134.88	121.70
1	A	155	TYR	C-N-CA	7.32	134.88	121.70
1	B	487	PHE	CA-CB-CG	7.06	120.86	113.80
1	A	2	ASP	CA-CB-CG	6.98	119.58	112.60
1	A	212	GLY	CA-C-N	-6.81	112.06	120.64
1	A	212	GLY	C-N-CA	-6.81	112.06	120.64
1	B	374	GLU	CA-C-N	6.58	127.61	120.44
1	B	374	GLU	C-N-CA	6.58	127.61	120.44
1	A	141	GLU	CA-C-N	6.51	130.26	120.75
1	A	141	GLU	C-N-CA	6.51	130.26	120.75
1	A	212	GLY	O-C-N	-6.17	115.21	122.50
1	A	30	VAL	CA-C-N	-6.03	112.80	121.42
1	A	30	VAL	C-N-CA	-6.03	112.80	121.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	VAL	O-C-N	-5.97	116.22	122.25
1	A	34	GLY	CA-C-N	-5.96	114.36	122.77
1	A	34	GLY	C-N-CA	-5.96	114.36	122.77
1	B	419	ASN	CA-CB-CG	5.92	118.52	112.60
1	A	132	GLY	CA-C-O	-5.74	115.90	121.86
1	A	205	VAL	N-CA-C	-5.73	105.14	110.53
1	A	107	ASP	CA-CB-CG	5.69	118.29	112.60
1	A	41	PRO	CA-C-N	5.68	129.97	122.42
1	A	41	PRO	C-N-CA	5.68	129.97	122.42
1	B	451	ASN	CA-CB-CG	-5.68	106.92	112.60
1	A	187	PHE	CA-C-N	5.66	130.75	122.77
1	A	187	PHE	C-N-CA	5.66	130.75	122.77
1	B	403	PHE	CA-CB-CG	5.65	119.45	113.80
1	A	139	ARG	NE-CZ-NH1	-5.64	115.86	121.50
1	A	237	VAL	CA-C-O	-5.62	114.61	120.51
1	A	94	ILE	O-C-N	5.61	126.45	121.57
1	B	347	ARG	CD-NE-CZ	5.60	132.25	124.40
1	B	536	ILE	O-C-N	5.55	129.42	123.03
1	A	145	ALA	CA-C-N	-5.55	113.63	122.29
1	A	145	ALA	C-N-CA	-5.55	113.63	122.29
1	A	153	ILE	CA-C-N	-5.31	112.41	121.97
1	A	153	ILE	C-N-CA	-5.31	112.41	121.97
1	B	519	ASP	CA-CB-CG	-5.30	107.30	112.60
1	A	61	ARG	CD-NE-CZ	5.26	131.77	124.40
1	A	86	GLY	CA-C-O	5.25	124.55	118.98
1	A	4	ARG	CA-C-N	-5.19	112.93	120.29
1	A	4	ARG	C-N-CA	-5.19	112.93	120.29
1	A	229	ASP	CA-C-N	-5.15	111.71	121.54
1	A	229	ASP	C-N-CA	-5.15	111.71	121.54
1	A	243	LEU	CA-C-O	5.08	125.55	119.60
1	A	184	PHE	CA-CB-CG	-5.05	108.75	113.80

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	98	0
1	B	1966	0	1946	87	0
2	A	70	0	0	3	0
2	B	66	0	0	3	0
All	All	4068	0	3895	181	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 23.

All (181) 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:335:MET:HE2	1:B:339:GLY:O	1.87	0.74
1:A:65:VAL:HG11	1:A:228:PHE:O	1.88	0.74
1:B:337:LYS:HD2	1:B:370:GLY:HA3	1.68	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:24:MET:HE2	1:A:29:ARG:HA	1.74	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:33:VAL:HG11	2:A:1101:HOH:O	1.98	0.64
1:A:193:GLY:O	1:A:195:MET:HG2	1.97	0.64
1:A:219:ASP:OD1	1:A:221:GLU:HG3	1.98	0.64
1:B:367:GLU:HG3	1:B:499:TYR:CE1	2.33	0.64
1:B:429:ASP:O	1:B:510:LYS:HD2	1.98	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:A:47:ARG:HA	1:A:68:GLU:OE1	1.99	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ILE:HD12	1:B:468:ILE:HG13	1.81	0.61
1:B:505:VAL:HG13	1:B:515:VAL:HG11	1.82	0.61
1:A:118:TYR:HD2	1:A:120:LEU:HD23	1.67	0.60
1:A:146:GLU:HG2	1:A:246:LYS:HZ2	1.65	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:HG2	1:A:146:GLU:O	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: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:194:LYS:O	1:A:195:MET:HE2	2.07	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:A:37:LYS:HG3	1:A:70:GLY:CA	2.39	0.53
1:B:407:ASP:OD1	1:B:527:LYS:NZ	2.41	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:A:197:ARG:HG3	1:A:233:ARG:HD3	1.92	0.50
1:B:366:THR:O	1:B:370:GLY:HA2	2.11	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:312:GLU:OE2	1:B:356:ILE:HD12	2.12	0.49
1:B:501:ALA:O	1:B:505:VAL:HG23	2.13	0.49
1:A:228:PHE:O	1:A:229:ASP:O	2.29	0.49
1:A:12:GLU:HG2	2:A:1065:HOH:O	2.11	0.49
1:A:37:LYS:HB2	1:A:67:GLU:O	2.12	0.49
1:A:197:ARG:HD3	1:A:199:TYR:CZ	2.48	0.49
1:A:233:ARG:C	1:A:234:LEU:HD23	2.38	0.49
1:B:325:PRO:HG2	1:B:328:GLU:HG2	1.94	0.49
1:B:371:VAL:O	1:B:372:LEU:HD23	2.12	0.49
1:A:131:SER:HG	1:A:134:TYR:HH	1.52	0.49
1:B:435:ARG:HB2	1:B:440:ILE:HG21	1.94	0.49
1:A:8:ARG:O	1:A:12:GLU:HG3	2.13	0.48
1:B:318:ARG:HA	1:B:420:LEU:HD22	1.95	0.48
1:A:249:GLU:O	1:A:252:LYS:HB2	2.14	0.48
1:A:146:GLU:CD	1:A:242:LYS:HD3	2.38	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: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:194:LYS:O	1:A:233:ARG:HB2	2.15	0.47
1:B:465:ARG:HH11	1:B:465:ARG:HG3	1.80	0.47
1:B:494:LYS:O	1:B:533:ARG:HD2	2.14	0.47
1:A:195:MET:HE2	1:A:195:MET:HA	1.97	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:A:194:LYS:HG2	1:A:235:ASN:HD21	1.79	0.46
1:B:408:LYS:HE2	1:B:527:LYS:HD3	1.96	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:301:MET:HE3	1:B:377:VAL:HG11	1.99	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: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:340:THR:HB	1:B:341:PRO:HD2	1.98	0.45
1:B:487:PHE:C	1:B:488:LEU:HD12	2.42	0.45
1:A:29:ARG:O	1:A:43:LYS:HB3	2.17	0.44
1:A:194:LYS:C	1:A:195:MET:HE2	2.43	0.44
1:B:438:GLU:HG3	1:B:439:ARG:O	2.18	0.44
1:B:495:MET:N	2:B:1011:HOH:O	2.50	0.44
1:B:416:TYR:CE2	1:B:418:TYR:HB2	2.53	0.44
1:B:517:GLU:HG2	1:B:523:LEU:HD21	1.99	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:13:ILE:HD11	1:A:57:LEU:HG	1.99	0.43
1:A:234:LEU:HD23	1:A:234:LEU:N	2.33	0.43
1:B:419:ASN:OD1	1:B:422:THR:HG23	2.18	0.43
1:B:443:SER:OG	1:B:445:ALA:HB2	2.18	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:385:ASP:O	1:B:397:TYR:HA	2.19	0.43
1:B:531:GLN:HB2	2:B:1104:HOH:O	2.18	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:LYS:N	1:B:524:GLY:O	2.49	0.43
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:OE2	1:A:232:GLU:HA	2.19	0.42
1:B:521:GLU:HG3	1:B:522:SER:N	2.33	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:465:ARG:HG3	1:B:465:ARG:NH1	2.34	0.42
1:B:494:LYS:NZ	1:B:517:GLU:OE2	2.52	0.42
1:A:218:LEU:HD12	1:A:218:LEU:HA	1.89	0.42
1:A:219:ASP:CG	1:A:221:GLU:HG3	2.45	0.42
1:A:148:LEU:HB3	1:A:162:PRO:HG2	2.00	0.41
1:A:166:MET:HE3	1:A:166:MET:HB2	1.85	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:35:MET:SD	1:A:39:GLY:HA2	2.61	0.41
1:A:158:ASP:OD1	1:A:158:ASP:N	2.53	0.41
1:B:514:LYS:O	1:B:538:ALA:HA	2.21	0.41
1:B:530:MET:HE3	1:B:530:MET:HB3	1.91	0.41
1:A:66:THR:HG21	1:A:81:LEU:HD23	2.04	0.41
1:A:108:LYS:HB3	1:A:110:LYS:HG2	2.03	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:94:ILE:HG12	1:B:478:PHE:CZ	2.56	0.40
1:A:181:ASP:HB3	1:A:183:SER:H	1.85	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%)	7	3
1	B	250/252 (99%)	239 (96%)	10 (4%)	1 (0%)	30	27
All	All	500/504 (99%)	473 (95%)	22 (4%)	5 (1%)	12	8

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%)	180 (88%)	24 (12%)	5	3
1	B	204/204 (100%)	178 (87%)	26 (13%)	4	2
All	All	408/408 (100%)	358 (88%)	50 (12%)	4	3

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	19	LYS
1	A	23	SER
1	A	50	GLU
1	A	55	GLU
1	A	74	GLU
1	A	76	ASP
1	A	119	ASN
1	A	126	TYR
1	A	131	SER
1	A	139	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	144	ASP
1	A	147	GLU
1	A	154	ILE
1	A	160	LYS
1	A	181	ASP
1	A	194	LYS
1	A	214	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	301	MET
1	B	303	GLU
1	B	340	THR
1	B	347	ARG
1	B	359	LYS
1	B	360	GLU
1	B	361	ARG
1	B	366	THR
1	B	371	VAL
1	B	399	VAL
1	B	403	PHE
1	B	406	SER
1	B	410	LYS
1	B	419	ASN
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	531	GLN
1	B	533	ARG
1	B	534	LEU
1	B	552	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	231	GLN
1	A	235	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 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 [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%)	-1.41	0 100 100	21, 36, 61, 120	0
1	B	252/252 (100%)	-1.41	0 100 100	22, 37, 58, 79	0
All	All	504/504 (100%)	-1.41	0 100 100	21, 36, 60, 120	0

There are no RSRZ outliers to report.

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.