Full wwPDB X-ray Structure Validation Report (i)

Feb 10, 2024 – 02:10 PM EST

PDB ID	:	2IFY
Title	:	Structure of Bacillus anthracis cofactor-independent phosphoglucerate mutase
Authors	:	Nukui, M.; Littlejohn, J.E.; Jedrzejas, M.J.
Deposited on	:	2006-09-21
Resolution	:	2.38 Å(reported)

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36
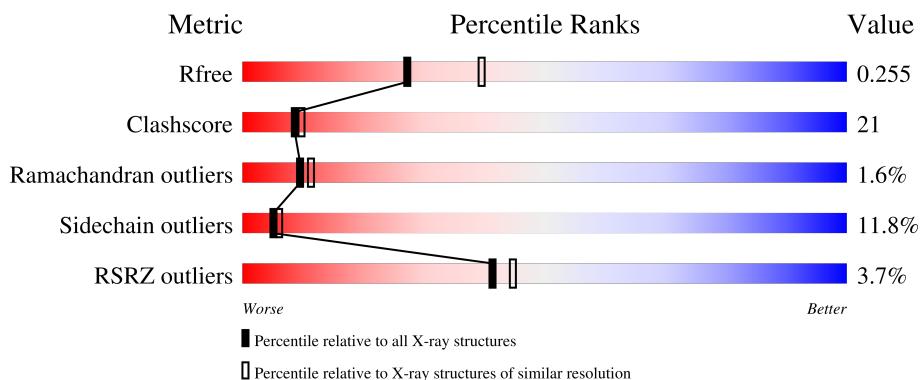
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
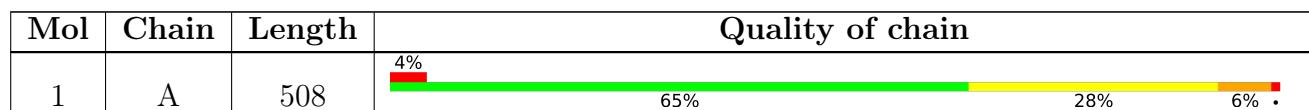
The reported resolution of this entry is 2.38 Å.

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	Percentile Ranks	Value
Rfree		0.255
Clashscore		21
Ramachandran outliers		1.6%
Sidechain outliers		11.8%
RSRZ outliers		3.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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 <=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	508	4% 65% 28% 6% ·

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4093 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 2,3-bisphosphoglycerate-independent phosphoglycerate mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	508	Total 3907	C 2461	N 661	O 765	S 20	0	0	0

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Mn 2	0	0
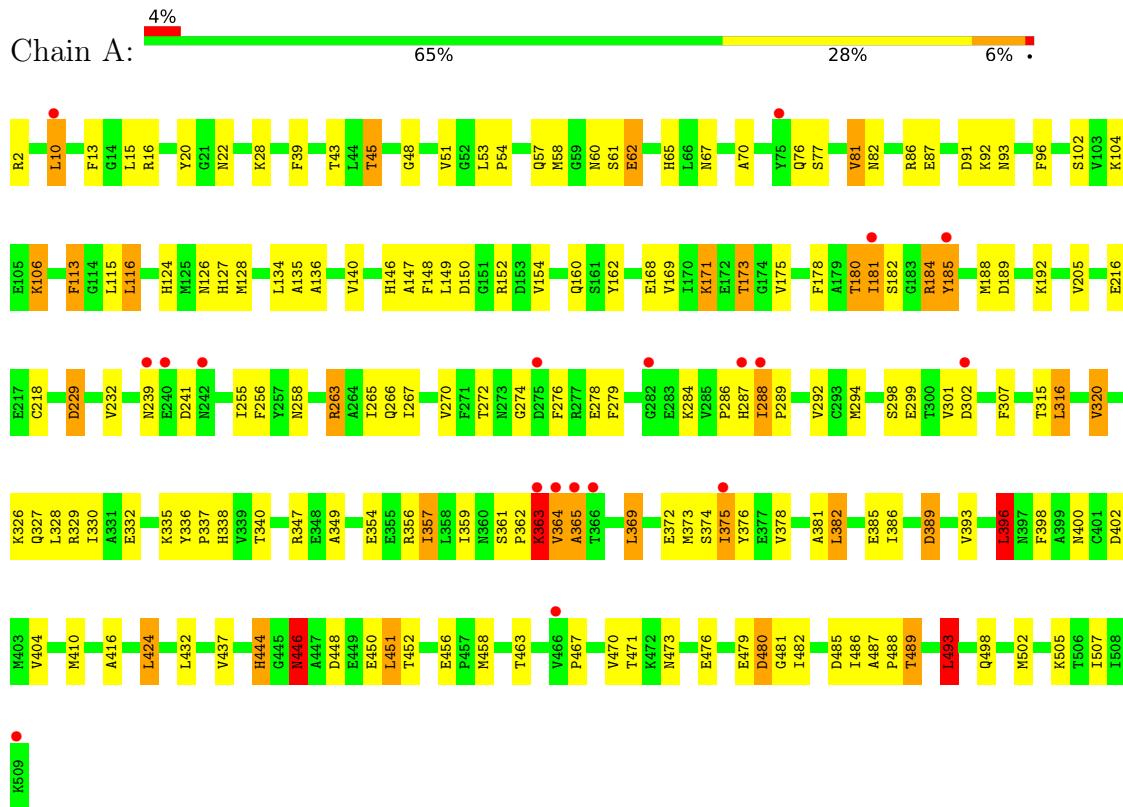
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	184	Total 184	O 184	0	0

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: 2,3-bisphosphoglycerate-independent phosphoglycerate mutase

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	43.62Å　72.74Å　185.18Å 90.00°　90.00°　90.00°	Depositor
Resolution (Å)	37.41　–　2.38 37.41　–　2.38	Depositor EDS
% Data completeness (in resolution range)	91.4 (37.41-2.38) 84.4 (37.41-2.38)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1, REFMAC	Depositor
R, R_{free}	0.245　,　0.298 0.256　,　0.255	Depositor DCC
R_{free} test set	1091 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	33.3	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 44.7	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	4093	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: MN

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	0.37	0/3986	0.73	3/5402 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	424	LEU	CA-CB-CG	6.04	129.20	115.30
1	A	493	LEU	CA-CB-CG	5.23	127.32	115.30
1	A	396	LEU	CA-CB-CG	5.17	127.19	115.30

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	3907	0	3775	158	0
2	A	2	0	0	0	0
3	A	184	0	0	23	0
All	All	4093	0	3775	158	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 21.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

All (158) 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:298:SER:O	1:A:301:VAL:HG22	1.60	1.02
1:A:404:VAL:HG11	1:A:416:ALA:CB	2.02	0.90
1:A:86:ARG:HG2	1:A:86:ARG:HH11	1.37	0.88
1:A:2:ARG:HH22	1:A:326:LYS:HG3	1.42	0.83
1:A:410:MET:CE	1:A:451:LEU:HD22	2.09	0.82
1:A:354:GLU:OE1	1:A:356:ARG:HD3	1.81	0.79
1:A:299:GLU:HG3	3:A:864:HOH:O	1.83	0.78
1:A:446:ASN:C	1:A:446:ASN:HD22	1.88	0.77
1:A:498:GLN:HG3	1:A:502:MET:HE2	1.65	0.77
1:A:320:VAL:HG21	1:A:393:VAL:HG11	1.66	0.76
1:A:410:MET:SD	3:A:816:HOH:O	2.43	0.75
1:A:410:MET:CG	3:A:816:HOH:O	2.37	0.73
1:A:404:VAL:HG11	1:A:416:ALA:HB3	1.71	0.72
1:A:288:ILE:H	1:A:289:PRO:HD3	1.55	0.72
1:A:288:ILE:N	1:A:289:PRO:HD3	2.04	0.72
1:A:54:PRO:HG2	1:A:57:GLN:HE21	1.55	0.72
1:A:169:VAL:O	1:A:173:THR:HB	1.89	0.72
1:A:410:MET:HG2	3:A:816:HOH:O	1.89	0.71
1:A:335:LYS:HA	1:A:338:HIS:HD2	1.56	0.71
1:A:302:ASP:HB2	3:A:784:HOH:O	1.91	0.70
1:A:239:ASN:O	1:A:241:ASP:O	2.10	0.69
1:A:192:LYS:H	1:A:266:GLN:HE22	1.41	0.68
1:A:362:PRO:HG3	1:A:373:MET:HA	1.76	0.67
1:A:51:VAL:HG12	1:A:51:VAL:O	1.94	0.67
1:A:289:PRO:HA	3:A:792:HOH:O	1.94	0.67
1:A:410:MET:HE1	1:A:451:LEU:HD22	1.75	0.67
1:A:82:ASN:OD1	1:A:127:HIS:HE1	1.78	0.67
1:A:340:THR:HG22	1:A:356:ARG:HD2	1.76	0.66
1:A:347:ARG:NH1	1:A:349:ALA:O	2.30	0.65
1:A:45:THR:HG23	1:A:482:ILE:HG22	1.78	0.64
1:A:381:ALA:O	1:A:385:GLU:HG2	1.96	0.64
1:A:363:LYS:HA	3:A:751:HOH:O	1.96	0.64
1:A:124:HIS:HD2	1:A:126:ASN:H	1.46	0.63
1:A:188:MET:O	1:A:263:ARG:HB2	1.99	0.63
1:A:135:ALA:HB1	1:A:140:VAL:CG2	2.29	0.62
1:A:20:TYR:OH	3:A:875:HOH:O	2.15	0.62
1:A:382:LEU:CD1	1:A:396:LEU:HG	2.29	0.62
1:A:332:GLU:HA	1:A:359:ILE:O	2.00	0.61
1:A:400:ASN:O	1:A:404:VAL:HG12	2.01	0.61
1:A:437:VAL:HG21	1:A:493:LEU:HG	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:LEU:HD11	1:A:181:ILE:HD13	1.82	0.60
1:A:382:LEU:HD23	1:A:386:ILE:HD11	1.83	0.59
1:A:382:LEU:HD13	1:A:396:LEU:HG	1.82	0.59
1:A:146:HIS:ND1	1:A:180:THR:HB	2.18	0.59
1:A:61:SER:O	1:A:65:HIS:HD2	1.86	0.58
1:A:189:ASP:HB2	3:A:874:HOH:O	2.02	0.58
1:A:2:ARG:NH2	1:A:326:LYS:HG3	2.18	0.57
1:A:86:ARG:HG2	1:A:86:ARG:NH1	2.13	0.57
1:A:320:VAL:HG21	1:A:393:VAL:CG1	2.34	0.57
1:A:149:LEU:HD12	1:A:232:VAL:HG21	1.85	0.57
1:A:487:ALA:HB3	1:A:488:PRO:HD3	1.87	0.57
1:A:276:PHE:HB2	3:A:787:HOH:O	2.04	0.57
1:A:180:THR:HG22	3:A:709:HOH:O	2.05	0.57
1:A:485:ASP:O	1:A:489:THR:HG22	2.05	0.56
1:A:302:ASP:O	1:A:302:ASP:OD2	2.23	0.56
1:A:480:ASP:OD2	1:A:480:ASP:N	2.33	0.56
1:A:113:PHE:HB3	1:A:146:HIS:HB2	1.88	0.56
1:A:327:GLN:HG3	1:A:354:GLU:HA	1.88	0.56
1:A:374:SER:O	1:A:378:VAL:HG23	2.07	0.54
1:A:53:LEU:HD23	1:A:76:GLN:OE1	2.08	0.54
1:A:364:VAL:HG13	1:A:369:LEU:HD11	1.89	0.54
1:A:51:VAL:HG13	1:A:67:ASN:OD1	2.07	0.54
1:A:328:LEU:HD11	1:A:357:ILE:HG23	1.90	0.54
1:A:288:ILE:N	1:A:289:PRO:CD	2.72	0.53
1:A:327:GLN:NE2	1:A:329:ARG:HE	2.07	0.53
1:A:2:ARG:NH2	1:A:326:LYS:HB2	2.25	0.52
1:A:488:PRO:HG3	1:A:502:MET:HE3	1.91	0.52
1:A:2:ARG:HH22	1:A:326:LYS:CG	2.20	0.52
1:A:330:ILE:HD12	1:A:357:ILE:HG12	1.91	0.52
1:A:10:LEU:O	1:A:398:PHE:O	2.28	0.52
1:A:149:LEU:CD1	1:A:181:ILE:HD13	2.39	0.52
1:A:58:MET:HG3	3:A:877:HOH:O	2.10	0.52
1:A:452:THR:OG1	1:A:456:GLU:HG2	2.10	0.51
1:A:446:ASN:C	1:A:446:ASN:ND2	2.63	0.51
1:A:330:ILE:HG21	1:A:382:LEU:HD12	1.92	0.51
1:A:102:SER:O	1:A:106:LYS:HB2	2.11	0.51
1:A:185:TYR:HB3	3:A:862:HOH:O	2.11	0.50
1:A:347:ARG:HG2	1:A:347:ARG:HH11	1.76	0.50
1:A:316:LEU:O	1:A:320:VAL:HG13	2.11	0.50
1:A:147:ALA:HB2	1:A:178:PHE:HE1	1.74	0.50
1:A:301:VAL:CG2	3:A:714:HOH:O	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ALA:HB1	1:A:140:VAL:HG21	1.93	0.50
1:A:327:GLN:HB3	1:A:393:VAL:HG13	1.93	0.50
1:A:365:ALA:CB	3:A:774:HOH:O	2.59	0.49
1:A:154:VAL:HG11	1:A:162:TYR:OH	2.13	0.49
1:A:184:ARG:O	1:A:188:MET:N	2.37	0.49
1:A:485:ASP:O	1:A:489:THR:CG2	2.60	0.49
1:A:160:GLN:HE22	1:A:216:GLU:HA	1.78	0.49
1:A:106:LYS:HE2	3:A:879:HOH:O	2.11	0.49
1:A:116:LEU:HD23	1:A:128:MET:HE3	1.94	0.49
1:A:330:ILE:HG13	1:A:357:ILE:HG13	1.95	0.49
1:A:363:LYS:NZ	3:A:725:HOH:O	2.46	0.49
1:A:274:GLY:N	3:A:787:HOH:O	2.37	0.48
1:A:124:HIS:CD2	1:A:126:ASN:HB2	2.49	0.48
1:A:81:VAL:HG12	1:A:307:PHE:CE1	2.48	0.48
1:A:301:VAL:HG23	3:A:714:HOH:O	2.12	0.48
1:A:192:LYS:H	1:A:266:GLN:NE2	2.11	0.48
1:A:488:PRO:HB3	1:A:498:GLN:NE2	2.30	0.47
1:A:113:PHE:O	1:A:256:PHE:HA	2.15	0.46
1:A:60:ASN:HD22	1:A:62:GLU:H	1.64	0.46
1:A:92:LYS:HG3	3:A:882:HOH:O	2.15	0.46
1:A:347:ARG:NH1	1:A:347:ARG:HG2	2.30	0.46
1:A:113:PHE:CB	1:A:146:HIS:HB2	2.45	0.46
1:A:115:LEU:HD11	1:A:150:ASP:HA	1.98	0.46
1:A:369:LEU:H	1:A:369:LEU:HD12	1.81	0.45
1:A:375:ILE:HD12	1:A:376:TYR:CD2	2.52	0.45
1:A:229:ASP:O	1:A:232:VAL:HG22	2.16	0.45
1:A:372:GLU:O	1:A:375:ILE:HG13	2.16	0.45
1:A:54:PRO:CG	1:A:57:GLN:HE21	2.28	0.45
1:A:48:GLY:HA2	1:A:54:PRO:O	2.17	0.44
1:A:70:ALA:HA	1:A:315:THR:HG22	1.99	0.44
1:A:489:THR:HG21	1:A:507:ILE:HG12	1.99	0.44
1:A:327:GLN:HE21	1:A:329:ARG:HE	1.65	0.44
1:A:61:SER:O	1:A:65:HIS:CD2	2.70	0.44
1:A:135:ALA:HB1	1:A:140:VAL:HG22	1.98	0.44
1:A:136:ALA:HB2	1:A:175:VAL:HG22	2.00	0.44
1:A:16:ARG:HB3	1:A:22:ASN:ND2	2.33	0.44
1:A:39:PHE:CG	1:A:471:THR:HA	2.53	0.44
1:A:335:LYS:HA	1:A:338:HIS:CD2	2.44	0.43
1:A:279:PHE:HB3	3:A:880:HOH:O	2.18	0.43
1:A:86:ARG:HH11	1:A:86:ARG:CG	2.19	0.43
1:A:267:ILE:O	1:A:270:VAL:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LEU:HD13	1:A:162:TYR:HB3	2.00	0.43
1:A:330:ILE:HD12	1:A:357:ILE:CG1	2.48	0.43
1:A:375:ILE:HG13	1:A:375:ILE:H	1.62	0.43
1:A:404:VAL:HG11	1:A:416:ALA:HB2	1.93	0.43
1:A:332:GLU:CD	1:A:374:SER:HB2	2.39	0.43
1:A:61:SER:HB2	1:A:338:HIS:CE1	2.54	0.43
1:A:93:ASN:HD22	1:A:96:PHE:H	1.65	0.43
1:A:256:PHE:CE1	1:A:258:ASN:HB2	2.54	0.43
1:A:287:HIS:O	1:A:288:ILE:HB	2.19	0.43
1:A:359:ILE:HG13	1:A:378:VAL:HA	2.00	0.42
1:A:51:VAL:O	1:A:51:VAL:CG1	2.65	0.42
1:A:284:LYS:O	1:A:286:PRO:HD3	2.19	0.42
1:A:340:THR:CG2	1:A:356:ARG:HD2	2.47	0.42
1:A:171:LYS:NZ	1:A:171:LYS:HB3	2.34	0.42
1:A:136:ALA:HB2	1:A:173:THR:HG23	2.01	0.42
1:A:255:ILE:HG12	1:A:292:VAL:HB	2.01	0.42
1:A:148:PHE:HA	1:A:182:SER:O	2.19	0.42
1:A:410:MET:SD	1:A:450:GLU:HB2	2.60	0.42
1:A:181:ILE:HG12	1:A:218:CYS:SG	2.60	0.41
1:A:389:ASP:OD2	1:A:389:ASP:N	2.53	0.41
1:A:116:LEU:CD2	1:A:128:MET:HE3	2.50	0.41
1:A:288:ILE:O	1:A:288:ILE:HG22	2.20	0.41
1:A:15:LEU:HD12	1:A:43:THR:HG22	2.01	0.41
1:A:15:LEU:HG	1:A:467:PRO:HD3	2.01	0.41
1:A:77:SER:O	1:A:81:VAL:HG22	2.21	0.41
1:A:86:ARG:NH1	1:A:87:GLU:OE2	2.53	0.41
1:A:272:THR:O	1:A:302:ASP:OD1	2.38	0.41
1:A:485:ASP:C	1:A:488:PRO:HD2	2.41	0.41
1:A:39:PHE:HB3	1:A:470:VAL:O	2.21	0.41
1:A:60:ASN:HB2	3:A:819:HOH:O	2.21	0.40
1:A:332:GLU:HG2	3:A:743:HOH:O	2.21	0.40
1:A:336:TYR:HB3	1:A:337:PRO:HD3	2.02	0.40
1:A:486:ILE:HA	1:A:489:THR:HG23	2.02	0.40
1:A:489:THR:O	1:A:493:LEU:HD22	2.21	0.40
1:A:400:ASN:H	1:A:400:ASN:HD22	1.69	0.40
1:A:402:ASP:OD1	1:A:444:HIS:HE1	2.04	0.40

There are no symmetry-related clashes.

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	506/508 (100%)	464 (92%)	34 (7%)	8 (2%)	9	11

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229	ASP
1	A	288	ILE
1	A	365	ALA
1	A	446	ASN
1	A	481	GLY
1	A	363	LYS
1	A	444	HIS
1	A	265	ILE

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	414/424 (98%)	365 (88%)	49 (12%)	5	6

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	13	PHE
1	A	28	LYS

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Mol	Chain	Res	Type
1	A	45	THR
1	A	62	GLU
1	A	81	VAL
1	A	91	ASP
1	A	104	LYS
1	A	106	LYS
1	A	113	PHE
1	A	116	LEU
1	A	134	LEU
1	A	152	ARG
1	A	168	GLU
1	A	171	LYS
1	A	173	THR
1	A	180	THR
1	A	181	ILE
1	A	184	ARG
1	A	185	TYR
1	A	205	VAL
1	A	263	ARG
1	A	278	GLU
1	A	294	MET
1	A	316	LEU
1	A	320	VAL
1	A	357	ILE
1	A	361	SER
1	A	363	LYS
1	A	364	VAL
1	A	369	LEU
1	A	375	ILE
1	A	382	LEU
1	A	389	ASP
1	A	396	LEU
1	A	424	LEU
1	A	432	LEU
1	A	446	ASN
1	A	448	ASP
1	A	451	LEU
1	A	458	MET
1	A	463	THR
1	A	473	ASN
1	A	476	GLU
1	A	479	GLU

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Mol	Chain	Res	Type
1	A	480	ASP
1	A	489	THR
1	A	493	LEU
1	A	505	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	60	ASN
1	A	65	HIS
1	A	67	ASN
1	A	93	ASN
1	A	124	HIS
1	A	127	HIS
1	A	225	ASN
1	A	249	ASN
1	A	266	GLN
1	A	287	HIS
1	A	296	HIS
1	A	322	GLN
1	A	327	GLN
1	A	338	HIS
1	A	388	ASN
1	A	446	ASN
1	A	473	ASN
1	A	498	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 ⓘ

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 ⓘ

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(Å²)	Q<0.9
1	A	508/508 (100%)	0.51	19 (3%)	41	45	28, 53, 64, 70	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	288	ILE	5.7
1	A	287	HIS	5.2
1	A	282	GLY	4.7
1	A	185	TYR	4.4
1	A	363	LYS	4.3
1	A	240	GLU	3.8
1	A	365	ALA	3.3
1	A	509	LYS	3.1
1	A	366	THR	3.1
1	A	466	VAL	3.0
1	A	10	LEU	2.8
1	A	375	ILE	2.5
1	A	275	ASP	2.4
1	A	242	ASN	2.2
1	A	181	ILE	2.2
1	A	75	TYR	2.2
1	A	302	ASP	2.1
1	A	364	VAL	2.0
1	A	239	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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, 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	B-factors(Å^2)	Q<0.9
2	MN	A	601	1/1	0.98	0.07	32,32,32,32	0
2	MN	A	701	1/1	0.99	0.07	29,29,29,29	0

6.5 Other polymers ⓘ

There are no such residues in this entry.