



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 05:04 PM UTC

PDB ID : 4FGW / pdb_00004fgw
Title : Structure of Glycerol-3-Phosphate Dehydrogenase, GPD1, from *Sacharomyces Cerevisiae*
Authors : Aparicio, D.; Munmun, N.; Carpena, X.; Fita, I.; Loewen, P.
Deposited on : 2012-06-05
Resolution : 2.45 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

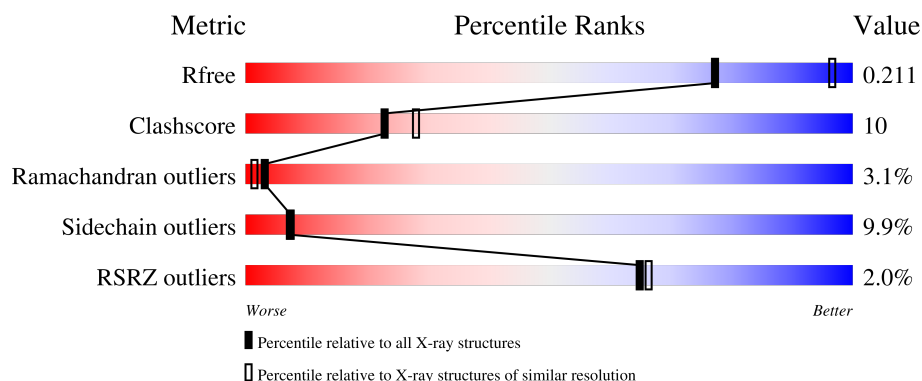
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	391	% 70% 14% 5% 10%
1	B	391	2% 72% 14% • 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5516 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 Glycerol-3-phosphate dehydrogenase [NAD(+)] 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	353	Total	C	N	O	S	0	0	0
			2731	1743	459	514	15			
1	B	353	Total	C	N	O	S	0	0	0
			2731	1743	459	514	15			

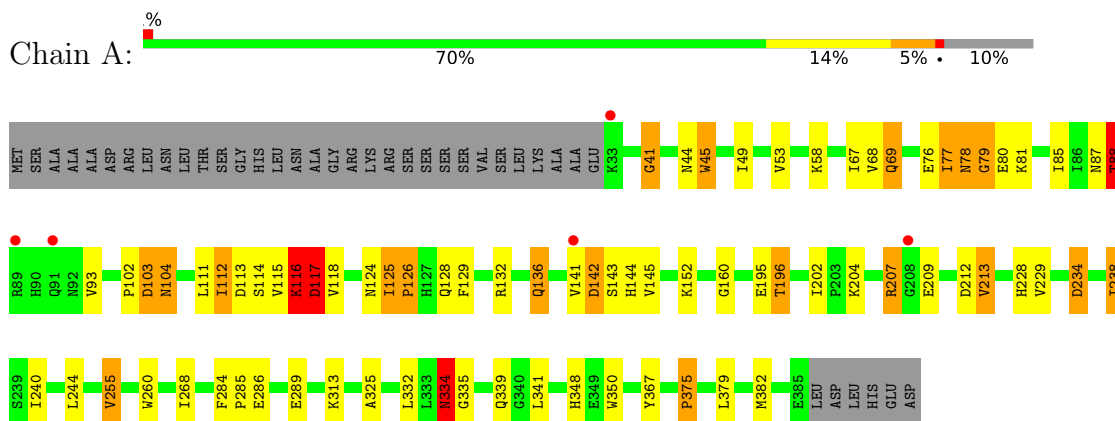
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	39	Total	O	0	0
			39	39		
2	B	15	Total	O	0	0
			15	15		

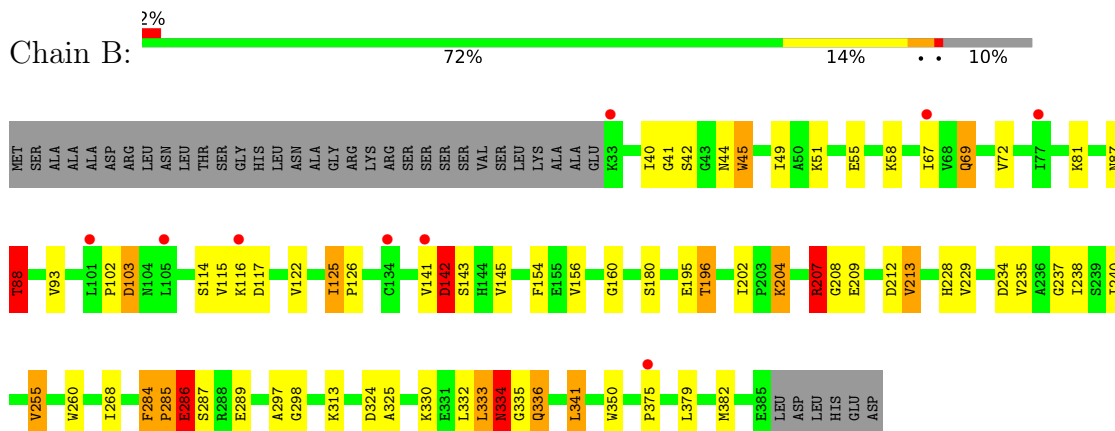
3 Residue-property plots [i](#)

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: Glycerol-3-phosphate dehydrogenase [NAD(+)] 1



- Molecule 1: Glycerol-3-phosphate dehydrogenase [NAD(+)] 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	64.42Å 64.42Å 198.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.40 – 2.45 29.40 – 2.46	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.40-2.45) 99.7 (29.40-2.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.53 (at 2.45Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.200 , 0.207 0.203 , 0.211	Depositor DCC
R_{free} test set	1492 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	54.2	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.057 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5516	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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	0.80	0/2791	1.40	15/3788 (0.4%)
1	B	0.81	0/2791	1.46	22/3788 (0.6%)
All	All	0.81	0/5582	1.43	37/7576 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	208	GLY	N-CA-C	12.11	129.53	112.82
1	B	207	ARG	N-CA-C	-11.41	89.32	108.26
1	B	285	PRO	N-CA-C	9.16	130.33	114.75
1	B	207	ARG	CB-CA-C	-8.77	96.63	110.14
1	B	285	PRO	CA-C-O	-6.72	109.38	118.78
1	A	289	GLU	CA-C-N	6.17	128.83	120.38
1	A	289	GLU	C-N-CA	6.17	128.83	120.38
1	B	289	GLU	CA-C-N	6.16	128.82	120.38
1	B	289	GLU	C-N-CA	6.16	128.82	120.38
1	A	334	ASN	CA-CB-CG	5.92	118.52	112.60
1	A	87	ASN	CA-C-N	5.92	132.84	121.54
1	A	87	ASN	C-N-CA	5.92	132.84	121.54
1	A	375	PRO	N-CA-C	5.86	124.55	112.47
1	B	375	PRO	N-CA-C	5.83	124.48	112.47
1	B	87	ASN	CA-C-N	5.82	132.66	121.54
1	B	87	ASN	C-N-CA	5.82	132.66	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	126	PRO	CA-C-N	5.78	128.29	120.38
1	B	126	PRO	C-N-CA	5.78	128.29	120.38
1	A	126	PRO	CA-C-N	5.56	128.00	120.38
1	A	126	PRO	C-N-CA	5.56	128.00	120.38
1	A	79	GLY	N-CA-C	-5.50	107.38	115.30
1	B	88	THR	CA-C-N	5.45	131.52	121.70
1	B	88	THR	C-N-CA	5.45	131.52	121.70
1	A	88	THR	CA-C-N	5.42	131.45	121.70
1	A	88	THR	C-N-CA	5.42	131.45	121.70
1	A	118	VAL	N-CA-C	-5.39	100.07	108.86
1	B	213	VAL	N-CA-CB	5.20	116.39	110.72
1	B	330	LYS	CA-C-N	5.17	127.21	120.28
1	B	330	LYS	C-N-CA	5.17	127.21	120.28
1	A	213	VAL	N-CA-CB	5.17	116.36	110.72
1	A	88	THR	CB-CA-C	5.16	120.69	110.42
1	B	237	GLY	CA-C-N	5.11	127.74	120.53
1	B	237	GLY	C-N-CA	5.11	127.74	120.53
1	B	88	THR	CB-CA-C	5.11	120.59	110.42
1	A	244	LEU	N-CA-C	5.08	117.55	111.71
1	B	298	GLY	CA-C-N	5.07	127.14	120.60
1	B	298	GLY	C-N-CA	5.07	127.14	120.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	284	PHE	Peptide

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	2731	0	2693	57	0
1	B	2731	0	2693	56	0
2	A	39	0	0	0	0
2	B	15	0	0	0	0
All	All	5516	0	5386	113	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 10.

All (113) 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:112:ILE:N	1:A:112:ILE:HD13	1.58	1.14
1:A:141:VAL:O	1:A:142:ASP:HB2	1.53	1.08
1:B:285:PRO:N	1:B:286:GLU:HB2	1.68	1.07
1:B:142:ASP:HB3	1:B:145:VAL:HG23	1.36	1.07
1:B:51:LYS:O	1:B:55:GLU:HG3	1.60	1.00
1:B:141:VAL:O	1:B:142:ASP:HB2	1.65	0.97
1:B:285:PRO:N	1:B:286:GLU:CB	2.30	0.95
1:A:112:ILE:N	1:A:112:ILE:CD1	2.30	0.91
1:B:334:ASN:ND2	1:B:335:GLY:H	1.69	0.90
1:A:348:HIS:CD2	1:A:367:TYR:CE2	2.61	0.88
1:A:112:ILE:HD13	1:A:112:ILE:H	1.36	0.87
1:A:78:ASN:OD1	1:A:78:ASN:N	2.06	0.85
1:A:142:ASP:CG	1:A:144:HIS:CD2	2.57	0.83
1:A:141:VAL:O	1:A:142:ASP:CB	2.28	0.82
1:A:142:ASP:OD1	1:A:144:HIS:HD2	1.64	0.81
1:B:334:ASN:CG	1:B:335:GLY:H	1.88	0.81
1:B:333:LEU:C	1:B:334:ASN:HD22	1.88	0.81
1:B:51:LYS:O	1:B:55:GLU:CG	2.28	0.81
1:B:285:PRO:CA	1:B:286:GLU:HB2	2.07	0.80
1:A:142:ASP:OD1	1:A:144:HIS:CD2	2.36	0.79
1:B:284:PHE:C	1:B:286:GLU:HB3	2.08	0.78
1:B:334:ASN:ND2	1:B:335:GLY:N	2.30	0.78
1:B:207:ARG:HG2	1:B:207:ARG:O	1.85	0.77
1:B:49:ILE:CD1	1:B:122:VAL:HG11	2.19	0.72
1:B:51:LYS:HG2	1:B:55:GLU:OE2	1.90	0.72
1:A:76:GLU:HA	1:A:80:GLU:O	1.90	0.71
1:A:111:LEU:HB3	1:A:112:ILE:HD13	1.72	0.71
1:A:348:HIS:CG	1:A:367:TYR:CE2	2.79	0.71
1:B:142:ASP:CB	1:B:145:VAL:HG23	2.20	0.70
1:A:207:ARG:HG2	1:A:212:ASP:HB2	1.76	0.68
1:B:207:ARG:HG2	1:B:212:ASP:HB2	1.76	0.67
1:A:284:PHE:O	1:A:286:GLU:N	2.30	0.65
1:A:348:HIS:NE2	1:A:367:TYR:HE2	1.95	0.65
1:A:78:ASN:ND2	1:A:80:GLU:OE1	2.31	0.63
1:B:285:PRO:N	1:B:286:GLU:HB3	2.11	0.63
1:B:285:PRO:CA	1:B:286:GLU:CB	2.77	0.62
1:B:324:ASP:OD1	1:B:324:ASP:C	2.41	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:GLN:HG2	1:A:129:PHE:CD2	2.38	0.59
1:B:334:ASN:CG	1:B:335:GLY:N	2.57	0.59
1:B:333:LEU:O	1:B:334:ASN:ND2	2.30	0.59
1:A:142:ASP:CG	1:A:144:HIS:NE2	2.60	0.59
1:B:141:VAL:O	1:B:142:ASP:CB	2.46	0.58
1:B:160:GLY:HA2	1:B:350:TRP:CZ3	2.41	0.56
1:A:142:ASP:HB3	1:A:145:VAL:HG23	1.87	0.55
1:A:132:ARG:O	1:A:136:GLN:HG3	2.07	0.55
1:B:49:ILE:CD1	1:B:122:VAL:CG1	2.85	0.55
1:A:160:GLY:HA2	1:A:350:TRP:CZ3	2.42	0.55
1:A:116:LYS:O	1:A:117:ASP:C	2.50	0.54
1:B:49:ILE:HD12	1:B:122:VAL:HG11	1.90	0.54
1:A:195:GLU:HG2	1:A:228:HIS:HB2	1.89	0.54
1:A:77:ILE:C	1:A:79:GLY:H	2.16	0.54
1:A:53:VAL:HG12	1:A:68:VAL:HG21	1.89	0.54
1:B:195:GLU:HG2	1:B:228:HIS:HB2	1.89	0.53
1:B:255:VAL:HG22	1:B:260:TRP:CE3	2.44	0.53
1:A:144:HIS:CD2	1:A:144:HIS:H	2.26	0.53
1:A:234:ASP:O	1:A:238:ILE:HG23	2.08	0.52
1:A:348:HIS:CE1	1:A:367:TYR:HE2	2.28	0.52
1:A:129:PHE:CD2	1:A:129:PHE:N	2.74	0.52
1:A:113:ASP:O	1:A:116:LYS:HB2	2.09	0.52
1:A:255:VAL:HG22	1:A:260:TRP:CE3	2.44	0.52
1:B:284:PHE:O	1:B:286:GLU:HB3	2.08	0.52
1:A:348:HIS:CG	1:A:367:TYR:CD2	2.99	0.51
1:B:207:ARG:O	1:B:207:ARG:CG	2.54	0.51
1:A:348:HIS:NE2	1:A:367:TYR:CE2	2.74	0.51
1:B:284:PHE:O	1:B:287:SER:HB2	2.11	0.51
1:A:313:LYS:HG2	1:A:332:LEU:HD13	1.93	0.51
1:B:51:LYS:CG	1:B:55:GLU:OE2	2.59	0.51
1:B:284:PHE:C	1:B:286:GLU:CB	2.76	0.51
1:A:128:GLN:HG2	1:A:129:PHE:CE2	2.47	0.50
1:B:40:ILE:O	1:B:125:ILE:HG23	2.11	0.50
1:A:142:ASP:CG	1:A:144:HIS:HE2	2.19	0.50
1:B:235:VAL:O	1:B:238:ILE:HG22	2.12	0.50
1:A:77:ILE:C	1:A:79:GLY:N	2.70	0.49
1:A:41:GLY:HA2	1:A:125:ILE:HG22	1.93	0.49
1:A:78:ASN:C	1:A:80:GLU:H	2.20	0.49
1:A:116:LYS:O	1:A:117:ASP:O	2.30	0.48
1:B:41:GLY:O	1:B:42:SER:OG	2.30	0.48
1:A:348:HIS:CE1	1:A:367:TYR:CE2	3.00	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:ARG:O	1:B:212:ASP:HB2	2.13	0.48
1:B:41:GLY:C	1:B:42:SER:OG	2.57	0.47
1:B:333:LEU:O	1:B:334:ASN:C	2.56	0.47
1:A:78:ASN:C	1:A:80:GLU:N	2.72	0.47
1:B:379:LEU:HA	1:B:382:MET:HE3	1.96	0.47
1:A:325:ALA:HB1	1:A:341:LEU:HD21	1.96	0.47
1:B:313:LYS:HG2	1:B:332:LEU:HD13	1.97	0.47
1:A:379:LEU:HA	1:A:382:MET:HE3	1.95	0.46
1:B:238:ILE:HG13	1:B:297:ALA:CB	2.45	0.46
1:A:45:TRP:HB3	1:A:124:ASN:HD21	1.80	0.46
1:A:126:PRO:HD2	1:A:129:PHE:CD1	2.50	0.46
1:B:142:ASP:HB3	1:B:145:VAL:CG2	2.25	0.46
1:A:196:THR:HG22	1:A:229:VAL:HG22	1.98	0.46
1:A:111:LEU:HB3	1:A:112:ILE:CD1	2.43	0.46
1:B:69:GLN:HG2	1:B:114:SER:HA	1.98	0.45
1:A:69:GLN:HG2	1:A:114:SER:HA	1.98	0.45
1:A:334:ASN:CG	1:A:335:GLY:H	2.26	0.44
1:B:196:THR:HG22	1:B:229:VAL:HG22	1.98	0.44
1:A:104:ASN:OD1	1:A:104:ASN:N	2.37	0.44
1:B:333:LEU:C	1:B:334:ASN:ND2	2.67	0.43
1:A:77:ILE:HB	1:A:78:ASN:OD1	2.19	0.43
1:A:132:ARG:O	1:A:136:GLN:CG	2.67	0.42
1:A:111:LEU:C	1:A:112:ILE:HD13	2.35	0.42
1:A:45:TRP:HA	1:A:45:TRP:CE3	2.55	0.42
1:B:154:PHE:CE1	1:B:156:VAL:HB	2.55	0.42
1:B:204:LYS:H	1:B:204:LYS:HG2	1.54	0.42
1:B:51:LYS:O	1:B:55:GLU:HG2	2.17	0.41
1:A:80:GLU:HB3	1:A:85:ILE:HD11	2.03	0.41
1:B:45:TRP:HA	1:B:45:TRP:CE3	2.56	0.41
1:B:336:GLN:H	1:B:336:GLN:HG3	1.56	0.40
1:B:42:SER:HB3	1:B:72:VAL:HG22	2.04	0.40
1:B:180:SER:HB3	1:B:238:ILE:HG12	2.03	0.40
1:B:285:PRO:CD	1:B:286:GLU:HB2	2.48	0.40
1:B:284:PHE:HA	1:B:285:PRO:HD3	1.66	0.40
1:B:325:ALA:HB1	1:B:341:LEU:HD21	2.02	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	351/391 (90%)	318 (91%)	20 (6%)	13 (4%)	2	1
1	B	351/391 (90%)	322 (92%)	20 (6%)	9 (3%)	4	2
All	All	702/782 (90%)	640 (91%)	40 (6%)	22 (3%)	3	1

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	PRO
1	A	117	ASP
1	A	142	ASP
1	A	209	GLU
1	A	285	PRO
1	B	102	PRO
1	B	142	ASP
1	B	209	GLU
1	B	286	GLU
1	A	88	THR
1	A	103	ASP
1	A	234	ASP
1	B	88	THR
1	B	103	ASP
1	B	234	ASP
1	B	334	ASN
1	B	116	LYS
1	A	116	LYS
1	A	334	ASN
1	A	41	GLY
1	A	77	ILE
1	A	375	PRO

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	294/325 (90%)	263 (90%)	31 (10%)	6	6
1	B	294/325 (90%)	267 (91%)	27 (9%)	8	9
All	All	588/650 (90%)	530 (90%)	58 (10%)	7	7

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	45	TRP
1	A	49	ILE
1	A	58	LYS
1	A	67	ILE
1	A	69	GLN
1	A	78	ASN
1	A	81	LYS
1	A	88	THR
1	A	93	VAL
1	A	103	ASP
1	A	104	ASN
1	A	112	ILE
1	A	115	VAL
1	A	116	LYS
1	A	117	ASP
1	A	125	ILE
1	A	136	GLN
1	A	143	SER
1	A	152	LYS
1	A	196	THR
1	A	202	ILE
1	A	204	LYS
1	A	207	ARG
1	A	213	VAL
1	A	238	ILE
1	A	240	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	255	VAL
1	A	268	ILE
1	A	334	ASN
1	A	339	GLN
1	B	44	ASN
1	B	45	TRP
1	B	58	LYS
1	B	67	ILE
1	B	69	GLN
1	B	81	LYS
1	B	88	THR
1	B	93	VAL
1	B	103	ASP
1	B	115	VAL
1	B	117	ASP
1	B	125	ILE
1	B	142	ASP
1	B	143	SER
1	B	196	THR
1	B	202	ILE
1	B	204	LYS
1	B	207	ARG
1	B	213	VAL
1	B	240	ILE
1	B	255	VAL
1	B	268	ILE
1	B	286	GLU
1	B	333	LEU
1	B	334	ASN
1	B	336	GLN
1	B	341	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	124	ASN
1	A	144	HIS
1	A	281	GLN
1	A	378	ASN
1	B	44	ASN
1	B	108	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	124	ASN
1	B	192	HIS
1	B	263	ASN
1	B	269	GLN
1	B	281	GLN
1	B	334	ASN
1	B	378	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 [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	353/391 (90%)	0.12	5 (1%) 73 75	39, 78, 122, 146	0
1	B	353/391 (90%)	0.18	9 (2%) 58 61	36, 78, 146, 180	0
All	All	706/782 (90%)	0.15	14 (1%) 65 66	36, 78, 137, 180	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	116	LYS	3.3
1	B	141	VAL	3.2
1	A	208	GLY	2.9
1	B	33	LYS	2.6
1	B	101	LEU	2.6
1	A	33	LYS	2.4
1	B	375	PRO	2.3
1	B	77	ILE	2.1
1	A	89	ARG	2.1
1	B	105	LEU	2.1
1	A	141	VAL	2.1
1	B	67	ILE	2.1
1	A	91	GLN	2.1
1	B	134	CYS	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.