



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:56 PM UTC

PDB ID : 1R8W / pdb_00001r8w
Title : Native structure of the B12-independent glycerol dehydratase from clostridium butyricum
Authors : Lanzilotta, W.N.; Soucaille, P.; O'Brien, J.R.; Raynaud, C.
Deposited on : 2003-10-28
Resolution : 2.50 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

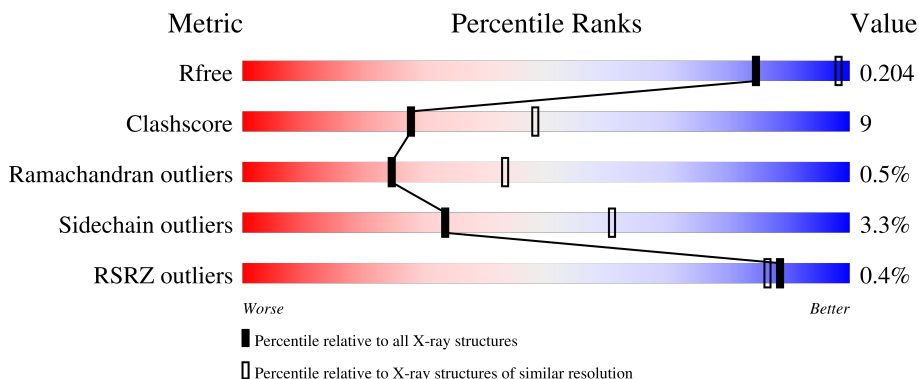
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	787	78% 19% .
1	B	787	76% 21% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12905 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 dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	786	Total	C	N	O	S	0	1	0
			6197	3918	1059	1194	26			
1	B	786	Total	C	N	O	S	0	1	0
			6197	3918	1059	1194	26			

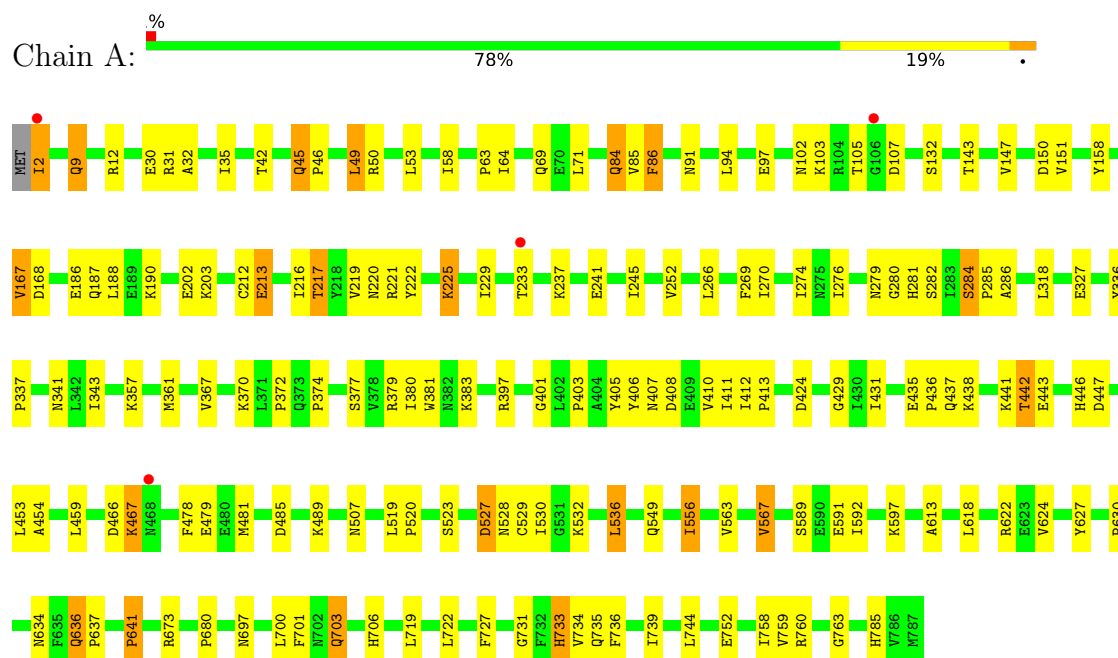
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	255	Total	O	0	0
			255	255		
2	B	256	Total	O	0	0
			256	256		

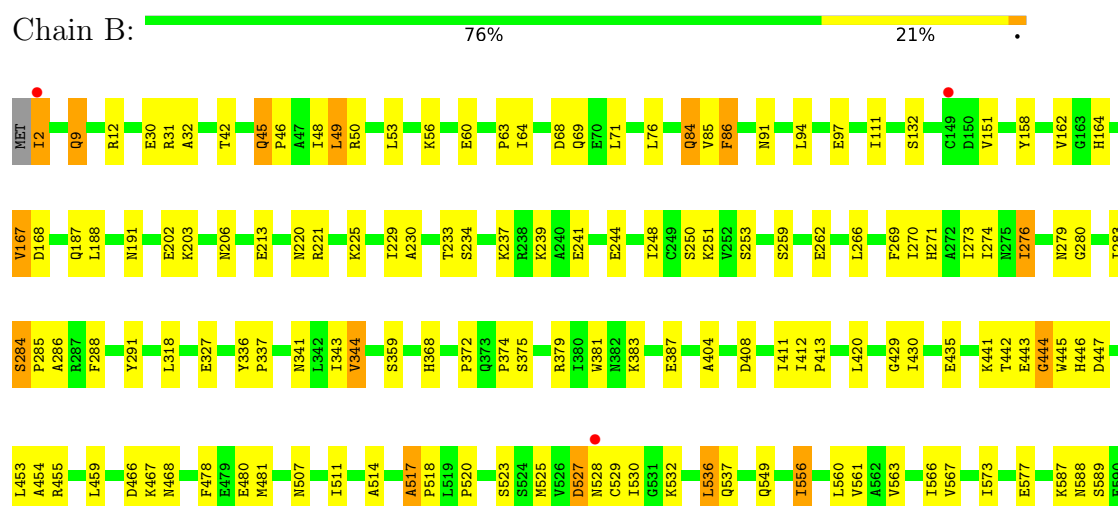
3 Residue-property plots

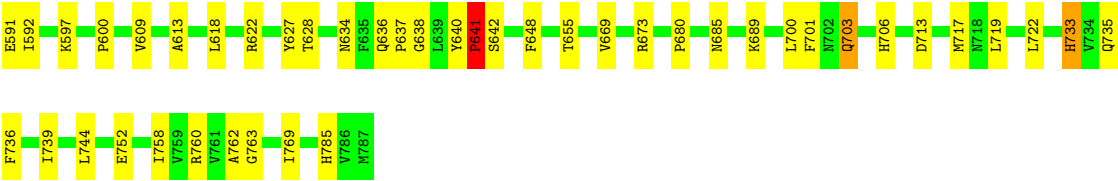
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: glycerol dehydratase



- Molecule 1: glycerol dehydratase





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	103.43Å 212.91Å 199.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.16 – 2.50 42.16 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.4 (42.16-2.50) 98.4 (42.16-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.05Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.171 , 0.203 0.172 , 0.204	Depositor DCC
R_{free} test set	4810 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtrriage
Anisotropy	0.264	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12905	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.5242e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.38	0/6319	0.90	24/8530 (0.3%)
1	B	0.38	0/6319	0.90	24/8530 (0.3%)
All	All	0.38	0/12638	0.90	48/17060 (0.3%)

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	527	ASP	N-CA-C	7.69	121.08	110.24
1	A	86	PHE	CA-C-N	7.60	127.64	119.28
1	A	86	PHE	C-N-CA	7.60	127.64	119.28
1	B	444	GLY	N-CA-C	7.55	124.02	114.66
1	B	627	TYR	N-CA-C	7.54	122.31	110.32
1	A	627	TYR	N-CA-C	7.17	121.71	110.17
1	A	527	ASP	N-CA-C	7.05	120.19	110.24
1	A	567	VAL	N-CA-C	6.92	117.88	111.45
1	B	280	GLY	N-CA-C	-6.78	102.32	111.54
1	B	706	HIS	N-CA-C	-6.70	101.62	109.93
1	A	706	HIS	N-CA-C	-6.55	101.81	109.93
1	B	151	VAL	N-CA-C	-6.46	106.66	111.90
1	A	411	ILE	N-CA-C	6.23	116.40	110.42
1	A	280	GLY	N-CA-C	-6.10	102.48	111.03
1	A	284	SER	N-CA-C	6.10	118.47	109.62
1	B	442	THR	N-CA-C	5.99	118.96	109.50
1	A	151	VAL	N-CA-C	-5.94	107.09	111.90
1	A	736	PHE	N-CA-C	5.90	119.10	109.24
1	A	71	LEU	N-CA-C	-5.88	106.65	113.88
1	B	411	ILE	N-CA-C	5.78	115.97	110.42
1	A	442	THR	N-CA-C	5.77	118.62	109.50
1	A	731	GLY	N-CA-C	-5.73	104.34	112.37
1	B	429	GLY	N-CA-C	-5.63	102.92	111.14
1	B	284	SER	N-CA-C	5.63	117.78	109.62
1	B	276	ILE	N-CA-C	-5.62	106.97	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	401	GLY	N-CA-C	-5.59	107.94	115.21
1	B	71	LEU	N-CA-C	-5.54	106.20	113.12
1	B	736	PHE	N-CA-C	5.43	118.09	109.50
1	A	613	ALA	N-CA-C	-5.41	105.47	111.36
1	A	286	ALA	CB-CA-C	-5.37	110.40	116.63
1	B	613	ALA	N-CA-C	-5.34	105.54	111.36
1	A	105	THR	N-CA-C	-5.29	105.96	112.90
1	A	429	GLY	N-CA-C	-5.29	103.42	111.14
1	A	150	ASP	N-CA-C	5.29	118.69	111.39
1	B	84	GLN	N-CA-C	-5.27	102.95	110.59
1	A	84	GLN	N-CA-C	-5.22	103.02	110.59
1	B	86	PHE	CA-C-N	5.20	124.87	119.56
1	B	86	PHE	C-N-CA	5.20	124.87	119.56
1	A	636	GLN	CA-C-N	5.19	125.09	119.85
1	A	636	GLN	C-N-CA	5.19	125.09	119.85
1	B	517	ALA	N-CA-C	5.10	116.90	109.30
1	B	640	TYR	CA-C-N	-5.10	113.47	119.84
1	B	640	TYR	C-N-CA	-5.10	113.47	119.84
1	B	655	THR	CA-C-N	5.09	126.20	119.84
1	B	655	THR	C-N-CA	5.09	126.20	119.84
1	B	286	ALA	CB-CA-C	-5.06	110.76	116.63
1	A	276	ILE	N-CA-C	-5.04	107.48	111.81
1	B	566	ILE	N-CA-C	5.03	117.38	111.09

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	6197	0	6130	104	0
1	B	6197	0	6130	118	0
2	A	255	0	0	5	0
2	B	256	0	0	3	0
All	All	12905	0	12260	222	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 9.

All (222) 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:42:THR:O	1:A:50:ARG:HD3	1.78	0.83
1:B:31:ARG:HB3	1:B:84:GLN:HG3	1.65	0.78
1:A:252:VAL:HG13	1:A:266:LEU:HD13	1.66	0.77
1:A:31:ARG:HB3	1:A:84:GLN:HG3	1.67	0.76
1:B:739:ILE:HD12	1:B:744:LEU:HD11	1.66	0.76
1:A:357:LYS:HG3	1:A:361:MET:HE2	1.66	0.75
1:B:42:THR:O	1:B:50:ARG:HD3	1.87	0.75
1:A:97:GLU:CD	1:A:327:GLU:HG3	2.13	0.73
1:B:30:GLU:HG2	1:B:63:PRO:HG2	1.70	0.72
1:B:478:PHE:HA	1:B:481:MET:HE3	1.71	0.72
1:B:97:GLU:CD	1:B:327:GLU:HG3	2.13	0.72
1:B:528:ASN:HB3	1:B:532:LYS:HE3	1.71	0.71
1:A:739:ILE:HD13	1:A:744:LEU:HD21	1.73	0.70
1:B:230:ALA:O	1:B:233:THR:HG22	1.93	0.69
1:B:597:LYS:NZ	1:B:597:LYS:HB3	2.08	0.68
1:A:2:ILE:N	1:A:2:ILE:HD12	2.09	0.68
1:B:600:PRO:HB2	1:B:609:VAL:CG2	2.25	0.66
1:B:188:LEU:HD11	1:B:202:GLU:HG3	1.78	0.66
1:B:523:SER:HA	1:B:536:LEU:HD22	1.78	0.66
1:A:343:ILE:HD11	1:A:379:ARG:HG3	1.79	0.65
1:B:167:VAL:HG22	1:B:525:MET:HB2	1.79	0.65
1:A:45:GLN:HG2	1:A:49:LEU:HB3	1.78	0.65
1:B:64:ILE:CD1	1:B:221:ARG:HB3	2.27	0.64
1:A:597:LYS:NZ	1:A:597:LYS:HB3	2.14	0.63
1:A:397:ARG:HD2	2:A:864:HOH:O	1.97	0.63
1:B:45:GLN:HG3	1:B:46:PRO:HD2	1.80	0.63
1:B:162:VAL:O	1:B:164:HIS:HD2	1.81	0.62
1:B:412:ILE:HB	1:B:413:PRO:HD3	1.79	0.62
1:B:30:GLU:HG2	1:B:63:PRO:CG	2.29	0.62
1:A:31:ARG:CB	1:A:84:GLN:HG3	2.29	0.62
1:B:381:TRP:CZ2	1:B:383:LYS:HB2	2.35	0.62
1:B:9:GLN:HG2	1:B:368:HIS:O	2.00	0.62
1:A:229:ILE:O	1:A:233:THR:HG23	2.01	0.61
1:A:372:PRO:HG3	1:A:758:ILE:HD12	1.83	0.61
1:A:528:ASN:HB3	1:A:532:LYS:HE3	1.82	0.61
1:A:42:THR:OG1	1:A:50:ARG:HD2	2.01	0.60
1:B:225:LYS:O	1:B:229:ILE:HG12	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:THR:HG21	2:A:919:HOH:O	2.02	0.60
1:A:523:SER:HA	1:A:536:LEU:HD22	1.83	0.60
1:B:680:PRO:HG3	1:B:785:HIS:HB3	1.84	0.60
1:B:752:GLU:CD	1:B:752:GLU:H	2.10	0.59
1:A:30:GLU:HG2	1:A:63:PRO:HG2	1.83	0.59
1:A:680:PRO:HG3	1:A:785:HIS:HB3	1.85	0.59
1:A:700:LEU:HA	1:A:733:HIS:CD2	2.37	0.59
1:A:318:LEU:HD13	1:A:374:PRO:HB3	1.85	0.58
1:A:343:ILE:CD1	1:A:379:ARG:HG3	2.34	0.58
1:A:64:ILE:HD12	1:A:222:TYR:CE1	2.38	0.58
1:A:412:ILE:HB	1:A:413:PRO:HD3	1.86	0.57
1:B:2:ILE:HD12	1:B:2:ILE:N	2.20	0.56
1:B:700:LEU:HD11	1:B:763:GLY:N	2.20	0.56
1:A:454:ALA:HA	1:A:556:ILE:HD11	1.86	0.56
1:B:271:HIS:CE1	1:B:283:ILE:HG22	2.40	0.56
1:B:454:ALA:HA	1:B:556:ILE:HD11	1.88	0.56
1:B:507:ASN:O	1:B:511:ILE:HG12	2.06	0.56
1:A:45:GLN:HG3	1:A:46:PRO:HD2	1.87	0.56
1:A:527:ASP:O	1:A:528:ASN:HB2	2.06	0.55
1:B:739:ILE:CD1	1:B:744:LEU:HD11	2.36	0.55
1:B:701:PHE:H	1:B:733:HIS:CD2	2.25	0.54
1:B:561:VAL:HG21	1:B:609:VAL:HG22	1.90	0.54
1:A:735:GLN:NE2	1:A:760:ARG:HH21	2.06	0.54
1:A:86:PHE:CE1	1:A:279:ASN:HB3	2.42	0.54
1:A:701:PHE:H	1:A:733:HIS:CD2	2.26	0.54
1:B:529:CYS:SG	1:B:536:LEU:HD13	2.48	0.54
1:B:56:LYS:O	1:B:60:GLU:HG3	2.08	0.54
1:A:102:ASN:HB2	1:A:103:LYS:HE3	1.89	0.53
1:A:407:ASN:ND2	1:A:410:VAL:HG23	2.24	0.53
1:A:45:GLN:HG3	1:A:46:PRO:CD	2.38	0.53
1:B:45:GLN:HG3	1:B:46:PRO:CD	2.38	0.53
1:B:42:THR:OG1	1:B:50:ARG:HD2	2.08	0.53
1:B:573:ILE:HG22	1:B:577:GLU:HB2	1.89	0.53
1:A:752:GLU:H	1:A:752:GLU:CD	2.16	0.52
1:B:12:ARG:HD3	1:B:69:GLN:O	2.09	0.52
1:B:700:LEU:HA	1:B:733:HIS:CD2	2.44	0.52
1:B:735:GLN:NE2	1:B:760:ARG:HH21	2.06	0.52
1:A:700:LEU:HA	1:A:733:HIS:HD2	1.73	0.52
1:B:86:PHE:CE1	1:B:279:ASN:HB3	2.45	0.52
1:A:217:THR:O	1:A:221:ARG:HG3	2.09	0.52
1:B:443:GLU:HA	1:B:443:GLU:OE1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:700:LEU:HD11	1:A:763:GLY:N	2.25	0.52
1:A:381:TRP:HB3	1:A:408:ASP:HB2	1.92	0.52
1:B:45:GLN:HG2	1:B:49:LEU:HB3	1.92	0.51
1:B:733:HIS:HE1	1:B:735:GLN:NE2	2.08	0.51
1:B:435:GLU:HG2	1:B:446:HIS:HB3	1.92	0.51
1:A:336:TYR:N	1:A:337:PRO:CD	2.73	0.51
1:B:528:ASN:N	1:B:528:ASN:HD22	2.09	0.51
1:B:634:ASN:HB3	2:B:906:HOH:O	2.10	0.51
1:A:188:LEU:HD11	1:A:202:GLU:HG3	1.93	0.51
1:A:636:GLN:HG3	1:A:697:ASN:HB2	1.92	0.51
1:B:514:ALA:HA	1:B:537:GLN:HB3	1.92	0.51
1:A:12:ARG:HD3	1:A:69:GLN:O	2.11	0.50
1:B:685:ASN:O	1:B:689:LYS:HG3	2.11	0.50
1:B:233:THR:HG23	1:B:239:LYS:HB2	1.92	0.50
1:B:284:SER:HB3	1:B:341:ASN:O	2.12	0.50
1:B:673:ARG:HG2	2:B:824:HOH:O	2.10	0.50
1:A:336:TYR:N	1:A:337:PRO:HD3	2.27	0.50
1:A:30:GLU:HG2	1:A:63:PRO:CG	2.42	0.50
1:B:9:GLN:CD	1:B:9:GLN:H	2.18	0.50
1:B:251:LYS:C	1:B:253:SER:H	2.19	0.50
1:A:634:ASN:HB3	2:A:914:HOH:O	2.10	0.49
1:A:357:LYS:CG	1:A:361:MET:HE2	2.39	0.49
1:B:372:PRO:HG3	1:B:758:ILE:HD12	1.93	0.49
1:B:701:PHE:H	1:B:733:HIS:HD2	1.60	0.49
1:A:443:GLU:OE1	1:A:443:GLU:HA	2.12	0.49
1:A:9:GLN:CD	1:A:9:GLN:H	2.19	0.49
1:B:31:ARG:CB	1:B:84:GLN:HG3	2.38	0.49
1:B:703:GLN:HE22	1:B:722:LEU:HD21	1.77	0.49
1:B:164:HIS:HE1	2:B:788:HOH:O	1.96	0.48
1:A:591:GLU:HG2	1:A:592:ILE:N	2.28	0.48
1:B:343:ILE:CD1	1:B:379:ARG:HG3	2.42	0.48
1:A:381:TRP:CZ2	1:A:383:LYS:HB2	2.47	0.48
1:B:618:LEU:O	1:B:622:ARG:HG3	2.13	0.48
1:A:241:GLU:O	1:A:245:ILE:HG13	2.13	0.48
1:A:618:LEU:O	1:A:622:ARG:HG3	2.14	0.48
1:A:212:CYS:O	1:A:216:ILE:HG13	2.13	0.48
1:A:270:ILE:O	1:A:274:ILE:HG13	2.14	0.48
1:A:528:ASN:HD22	1:A:532:LYS:HE3	1.79	0.48
1:B:68:ASP:O	1:B:69:GLN:HB2	2.14	0.48
1:A:107:ASP:OD2	1:A:336:TYR:N	2.38	0.48
1:A:377:SER:HB3	1:A:406:TYR:CE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:LEU:HD21	1:B:206:ASN:HD21	1.79	0.47
1:B:344:VAL:HG13	1:B:359:SER:HB3	1.96	0.47
1:B:381:TRP:CH2	1:B:383:LYS:HB2	2.49	0.47
1:A:217:THR:HG22	2:A:989:HOH:O	2.15	0.47
1:B:700:LEU:HD11	1:B:762:ALA:C	2.40	0.47
1:A:431:ILE:HD13	1:A:437:GLN:HG2	1.95	0.47
1:A:529:CYS:SG	1:A:536:LEU:HD13	2.55	0.47
1:A:703:GLN:HE22	1:A:722:LEU:HD21	1.78	0.47
1:B:455:ARG:HH22	1:B:466:ASP:CG	2.22	0.47
1:A:701:PHE:H	1:A:733:HIS:HD2	1.62	0.46
1:B:343:ILE:HD11	1:B:379:ARG:HG3	1.97	0.46
1:B:187:GLN:HG3	1:B:530:ILE:HG22	1.98	0.46
1:A:453:LEU:C	1:A:556:ILE:HD11	2.41	0.46
1:A:377:SER:HB3	1:A:406:TYR:HE1	1.80	0.46
1:B:597:LYS:HB3	1:B:597:LYS:HZ2	1.79	0.46
1:A:624:VAL:HB	1:A:637:PRO:HG3	1.97	0.46
1:B:441:LYS:HG2	1:B:527:ASP:HB2	1.97	0.46
1:B:713:ASP:O	1:B:717:MET:HG2	2.16	0.45
1:B:336:TYR:N	1:B:337:PRO:CD	2.79	0.45
1:A:187:GLN:HG3	1:A:530:ILE:HG22	1.96	0.45
1:A:367:VAL:O	1:A:370:LYS:HE3	2.17	0.45
1:A:435:GLU:HA	1:A:436:PRO:HD3	1.80	0.45
1:B:381:TRP:HB3	1:B:408:ASP:HB2	1.98	0.45
1:B:203:LYS:HA	1:B:203:LYS:HD3	1.80	0.45
1:B:244:GLU:O	1:B:248:ILE:HD13	2.16	0.45
1:B:591:GLU:HG2	1:B:592:ILE:N	2.31	0.45
1:A:284:SER:HB3	1:A:341:ASN:O	2.16	0.45
1:A:454:ALA:HA	1:A:556:ILE:CD1	2.47	0.45
1:A:485:ASP:O	1:A:489:LYS:HG3	2.17	0.45
1:A:636:GLN:HA	1:A:637:PRO:HD3	1.79	0.45
1:B:447:ASP:HA	1:B:549:GLN:NE2	2.32	0.44
1:B:32:ALA:HB2	1:B:85:VAL:HB	1.99	0.44
1:B:318:LEU:HD13	1:B:374:PRO:HB3	2.00	0.44
1:A:507:ASN:OD1	1:A:630:PRO:HD3	2.17	0.44
1:A:203:LYS:HA	1:A:203:LYS:HD3	1.78	0.44
1:B:466:ASP:O	1:B:467:LYS:HB2	2.17	0.44
1:B:336:TYR:N	1:B:337:PRO:HD3	2.33	0.44
1:B:669:VAL:HG22	1:B:700:LEU:O	2.18	0.44
1:A:225:LYS:O	1:A:229:ILE:HG12	2.17	0.44
1:A:478:PHE:HA	1:A:481:MET:HE3	2.00	0.44
1:A:673:ARG:HG2	2:A:852:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:VAL:O	1:B:567:VAL:HB	2.18	0.43
1:A:424:ASP:OD1	1:A:438:LYS:HE2	2.18	0.43
1:A:143:THR:O	1:A:147:VAL:HG23	2.18	0.43
1:A:441:LYS:HG2	1:A:527:ASP:HB2	2.00	0.43
1:B:233:THR:HG21	1:B:239:LYS:HA	2.00	0.43
1:B:404:ALA:HB2	1:B:760:ARG:NH2	2.34	0.43
1:B:187:GLN:OE1	1:B:191:ASN:ND2	2.48	0.43
1:A:435:GLU:HG2	1:A:446:HIS:HB3	2.00	0.43
1:B:269:PHE:O	1:B:273:ILE:HG13	2.19	0.43
1:A:281:HIS:O	1:A:282:SER:HB2	2.19	0.43
1:A:447:ASP:HA	1:A:549:GLN:NE2	2.34	0.42
1:B:167:VAL:HG13	1:B:168:ASP:N	2.34	0.42
1:A:167:VAL:HG13	1:A:168:ASP:N	2.33	0.42
1:A:442:THR:HG22	1:A:443:GLU:N	2.34	0.42
1:A:563:VAL:O	1:A:567:VAL:HB	2.19	0.42
1:A:237:LYS:O	1:A:241:GLU:HG3	2.18	0.42
1:A:733:HIS:CG	1:A:734:VAL:N	2.87	0.42
1:B:167:VAL:HG22	1:B:525:MET:CB	2.46	0.42
1:A:86:PHE:CZ	1:A:279:ASN:HB3	2.54	0.42
1:B:45:GLN:HE21	1:B:45:GLN:HB2	1.67	0.42
1:A:466:ASP:O	1:A:467:LYS:HB2	2.20	0.42
1:B:518:PRO:O	1:B:520:PRO:HD3	2.19	0.42
1:B:250:SER:O	1:B:253:SER:HB2	2.20	0.42
1:B:259:SER:OG	1:B:262:GLU:HG3	2.19	0.42
1:B:341:ASN:HA	1:B:375:SER:HB2	2.01	0.42
1:B:517:ALA:N	1:B:518:PRO:HD3	2.35	0.42
1:A:407:ASN:HB2	1:A:727:PHE:CG	2.54	0.42
1:B:132:SER:HB3	1:B:158:TYR:O	2.19	0.42
1:B:739:ILE:HD12	1:B:744:LEU:CD1	2.44	0.42
1:A:284:SER:HA	1:A:285:PRO:HD3	1.89	0.41
1:B:549:GLN:OE1	1:B:638:GLY:HA3	2.20	0.41
1:B:48:ILE:HD13	1:B:518:PRO:HB2	2.02	0.41
1:B:111:ILE:HG23	1:B:111:ILE:O	2.20	0.41
1:B:237:LYS:O	1:B:241:GLU:HG3	2.20	0.41
1:A:32:ALA:HB2	1:A:85:VAL:HB	2.03	0.41
1:A:380:ILE:CD1	1:A:405:TYR:HD2	2.33	0.41
1:B:700:LEU:C	1:B:700:LEU:HD23	2.45	0.41
1:B:266:LEU:O	1:B:270:ILE:HG13	2.20	0.41
1:A:219:VAL:HG13	1:A:269:PHE:CE2	2.56	0.41
1:B:76:LEU:HD22	1:B:276:ILE:CG1	2.51	0.41
1:A:188:LEU:HD12	1:A:188:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:556:ILE:O	1:B:560:LEU:HG	2.21	0.41
1:B:636:GLN:HA	1:B:637:PRO:HD3	1.84	0.41
1:A:132:SER:HB3	1:A:158:TYR:O	2.21	0.41
1:A:213:GLU:O	1:A:217:THR:HG23	2.21	0.41
1:B:284:SER:HA	1:B:285:PRO:HD3	1.90	0.41
1:B:453:LEU:C	1:B:556:ILE:HD11	2.45	0.41
1:B:641:PRO:O	1:B:642:SER:HB3	2.21	0.41
1:B:769:ILE:HD12	1:B:769:ILE:C	2.45	0.41
1:A:733:HIS:HE1	1:A:735:GLN:NE2	2.18	0.41
1:B:387:GLU:H	1:B:387:GLU:CD	2.21	0.40
1:B:435:GLU:CG	1:B:446:HIS:HB3	2.51	0.40
1:B:444:GLY:O	1:B:445:TRP:C	2.63	0.40
1:A:49:LEU:HD13	1:A:49:LEU:HA	1.85	0.40
1:B:288:PHE:HA	1:B:291:TYR:CZ	2.57	0.40
1:A:35:ILE:HB	1:A:58:ILE:HD11	2.03	0.40
1:B:587:LYS:O	1:B:588:ASN:HB2	2.21	0.40
1:B:600:PRO:HB2	1:B:609:VAL:HG21	2.02	0.40
1:A:186:GLU:O	1:A:190:LYS:HG2	2.22	0.40
1:B:527:ASP:O	1:B:528:ASN:HB2	2.20	0.40
1:A:519:LEU:HA	1:A:520:PRO:HD3	1.88	0.40
1:B:270:ILE:O	1:B:274:ILE:HG13	2.21	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	785/787 (100%)	748 (95%)	33 (4%)	4 (0%)	24	43
1	B	785/787 (100%)	743 (95%)	38 (5%)	4 (0%)	24	43
All	All	1570/1574 (100%)	1491 (95%)	71 (4%)	8 (0%)	24	43

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	641	PRO
1	B	641	PRO
1	A	589	SER
1	A	91	ASN
1	A	467	LYS
1	B	91	ASN
1	B	234	SER
1	B	589	SER

5.3.2 Protein sidechains [i](#)

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	676/676 (100%)	655 (97%)	21 (3%)	35	62
1	B	676/676 (100%)	653 (97%)	23 (3%)	32	60
All	All	1352/1352 (100%)	1308 (97%)	44 (3%)	33	61

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

Mol	Chain	Res	Type
1	A	2	ILE
1	A	9	GLN
1	A	45	GLN
1	A	49	LEU
1	A	53	LEU
1	A	94	LEU
1	A	167	VAL
1	A	213	GLU
1	A	217	THR
1	A	220	ASN
1	A	225	LYS
1	A	403	PRO
1	A	459	LEU
1	A	479	GLU
1	A	536	LEU

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Mol	Chain	Res	Type
1	A	556	ILE
1	A	641	PRO
1	A	703	GLN
1	A	719	LEU
1	A	733	HIS
1	A	759	VAL
1	B	2	ILE
1	B	9	GLN
1	B	45	GLN
1	B	49	LEU
1	B	53	LEU
1	B	94	LEU
1	B	167	VAL
1	B	213	GLU
1	B	220	ASN
1	B	344	VAL
1	B	420	LEU
1	B	430	ILE
1	B	459	LEU
1	B	468	ASN
1	B	480	GLU
1	B	536	LEU
1	B	556	ILE
1	B	628	THR
1	B	641	PRO
1	B	648	PHE
1	B	703	GLN
1	B	719	LEU
1	B	733	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	45	GLN
1	A	102	ASN
1	A	206	ASN
1	A	220	ASN
1	A	308	GLN
1	A	382	ASN
1	A	437	GLN
1	A	468	ASN

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Mol	Chain	Res	Type
1	A	477	ASN
1	A	584	ASN
1	A	697	ASN
1	A	703	GLN
1	A	733	HIS
1	A	735	GLN
1	B	45	GLN
1	B	84	GLN
1	B	110	GLN
1	B	164	HIS
1	B	206	ASN
1	B	220	ASN
1	B	308	GLN
1	B	382	ASN
1	B	468	ASN
1	B	477	ASN
1	B	528	ASN
1	B	584	ASN
1	B	593	GLN
1	B	703	GLN
1	B	733	HIS
1	B	735	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	786/787 (99%)	-0.51	4 (0%)	87 85	11, 26, 47, 64	1 (0%)
1	B	786/787 (99%)	-0.51	3 (0%)	88 86	11, 26, 47, 62	1 (0%)
All	All	1572/1574 (99%)	-0.51	7 (0%)	88 86	11, 26, 47, 64	2 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ILE	3.9
1	B	2	ILE	3.5
1	A	468	ASN	2.5
1	A	233	THR	2.3
1	B	149	CYS	2.3
1	A	106	GLY	2.3
1	B	528	ASN	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.