



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:39 AM UTC

PDB ID : 1R9D / pdb_00001r9d
Title : Glycerol bound form of the B12-independent glycerol dehydratase from *Clostridium butyricum*
Authors : Lanzilotta, W.N.; O'Brien, J.R.; Raynaud, C.; Soucaille, P.
Deposited on : 2003-10-28
Resolution : 1.80 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
Mogul : 2022.3.0, CSD as543be (2022)
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

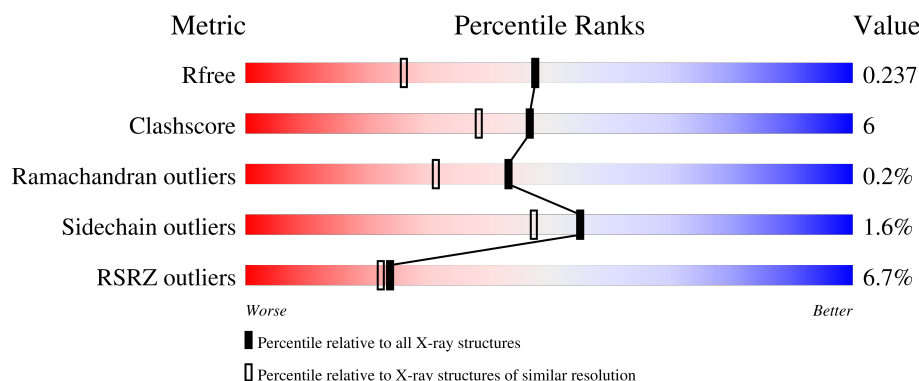
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	7% 82% 16% .
1	B	787	6% 85% 14% .

2 Entry composition [i](#)

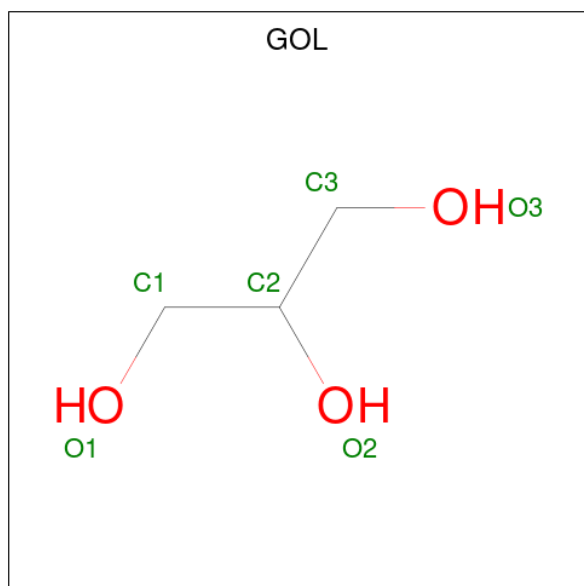
There are 3 unique types of molecules in this entry. The entry contains 13361 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	0	0
			6190	3915	1058	1192	25			
1	B	786	Total	C	N	O	S	0	0	0
			6190	3915	1058	1192	25			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

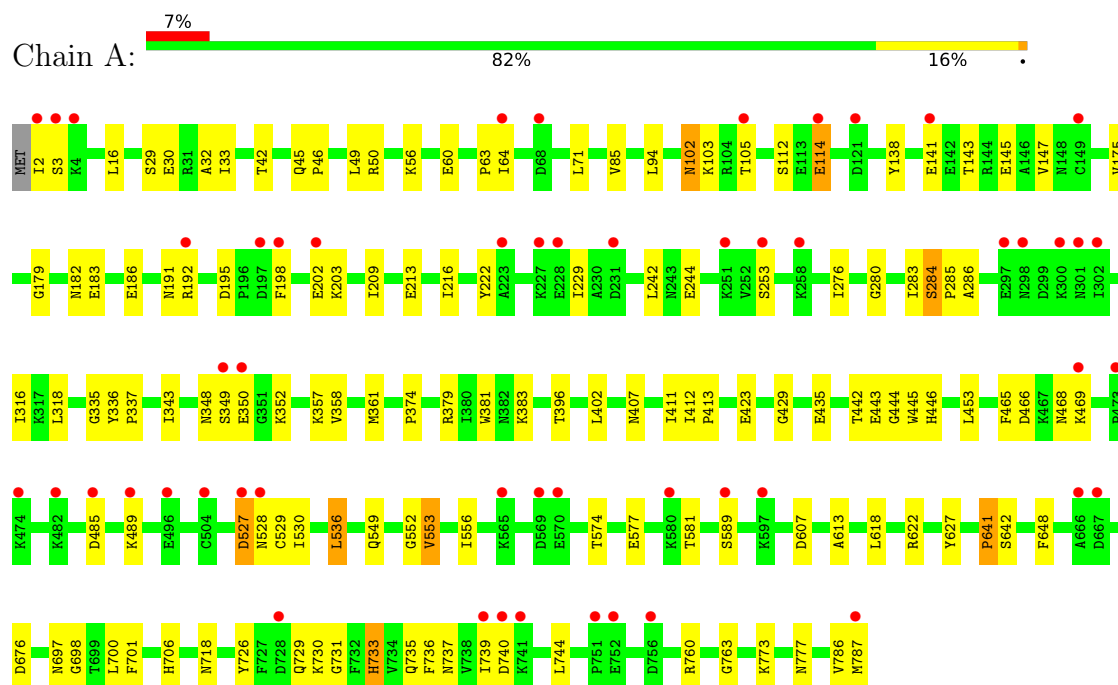
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	493	Total 493	O 493	0	0
3	B	476	Total 476	O 476	0	0

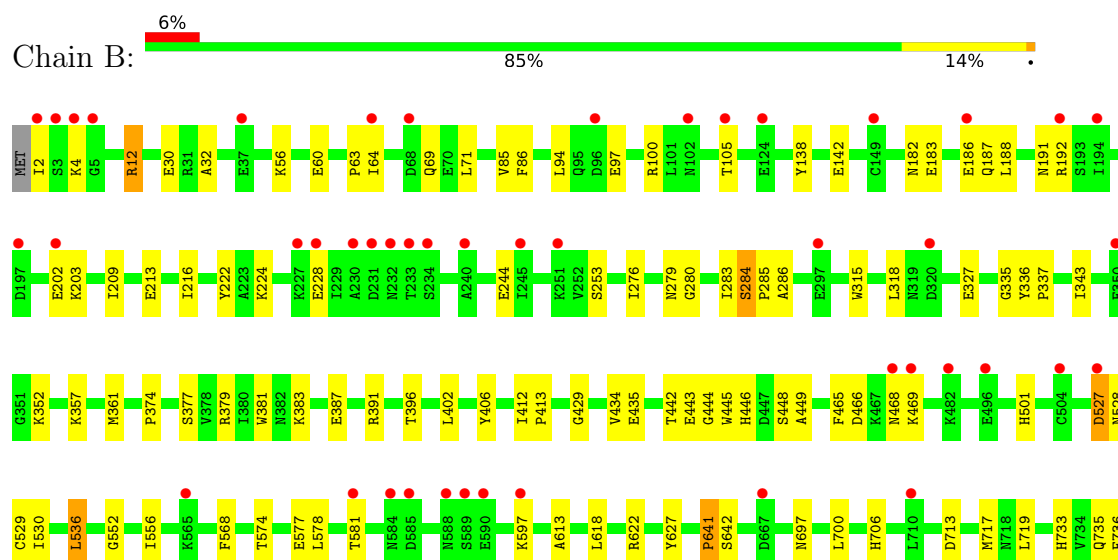
3 Residue-property plots [i](#)

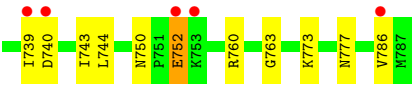
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 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	103.09Å 213.42Å 199.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.91 – 1.80 49.91 – 1.81	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.91-1.80) 99.4 (49.91-1.81)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 1.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.217 , 0.238 0.217 , 0.237	Depositor DCC
R_{free} test set	9995 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 30.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13361	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.17 % 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 7.7534e-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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	0.36	0/6312	0.88	24/8522 (0.3%)
1	B	0.36	0/6312	0.88	20/8522 (0.2%)
All	All	0.36	0/12624	0.88	44/17044 (0.3%)

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	527	ASP	N-CA-C	10.14	124.54	110.24
1	A	527	ASP	N-CA-C	9.78	124.03	110.24
1	B	613	ALA	N-CA-C	-6.95	103.79	111.36
1	A	706	HIS	N-CA-C	-6.82	101.17	109.83
1	A	613	ALA	N-CA-C	-6.75	104.00	111.36
1	A	446	HIS	N-CA-C	6.68	120.89	112.87
1	B	706	HIS	N-CA-C	-6.68	101.35	109.83
1	A	280	GLY	N-CA-C	-6.66	103.57	111.36
1	A	284	SER	N-CA-C	6.61	120.18	109.15
1	B	284	SER	N-CA-C	6.52	120.04	109.15
1	A	698	GLY	N-CA-C	6.48	120.21	111.72
1	B	627	TYR	N-CA-C	6.48	120.60	110.17
1	B	446	HIS	N-CA-C	6.45	120.61	112.87
1	B	280	GLY	N-CA-C	-6.44	102.78	111.54
1	B	442	THR	N-CA-C	6.37	119.89	109.24
1	A	442	THR	N-CA-C	6.33	119.51	109.50
1	B	283	ILE	N-CA-C	-6.22	98.59	107.98
1	A	411	ILE	N-CA-C	6.22	116.39	110.42
1	A	627	TYR	N-CA-C	6.20	120.15	110.17
1	A	71	LEU	N-CA-C	-5.97	106.53	113.88
1	B	71	LEU	N-CA-C	-5.97	106.13	113.41
1	A	283	ILE	N-CA-C	-5.94	98.93	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	553	VAL	N-CA-C	5.94	116.12	110.42
1	B	736	PHE	N-CA-C	5.85	119.01	109.24
1	A	736	PHE	N-CA-C	5.84	118.99	109.24
1	A	786	VAL	N-CA-C	-5.73	99.49	108.95
1	B	750	ASN	CA-C-N	5.66	125.12	119.24
1	B	750	ASN	C-N-CA	5.66	125.12	119.24
1	B	786	VAL	N-CA-C	-5.50	99.87	108.95
1	B	276	ILE	N-CA-C	-5.49	107.09	111.81
1	A	697	ASN	N-CA-C	-5.48	106.37	113.16
1	B	286	ALA	CB-CA-C	-5.41	110.36	116.63
1	A	429	GLY	N-CA-C	-5.33	103.36	111.14
1	A	737	ASN	N-CA-C	-5.24	101.17	109.76
1	A	286	ALA	CB-CA-C	-5.23	110.57	116.63
1	B	697	ASN	N-CA-C	-5.20	106.71	113.16
1	A	607	ASP	N-CA-C	5.18	116.93	111.28
1	A	549	GLN	N-CA-C	5.15	118.21	109.76
1	B	642	SER	CB-CA-C	-5.11	110.70	116.63
1	B	568	PHE	N-CA-C	5.10	118.66	112.23
1	A	642	SER	CB-CA-C	-5.08	110.74	116.63
1	A	407	ASN	N-CA-C	5.06	116.90	107.99
1	B	429	GLY	N-CA-C	-5.04	103.78	111.14
1	A	276	ILE	N-CA-C	-5.03	107.48	111.81

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	6190	0	6126	81	0
1	B	6190	0	6126	62	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
3	A	493	0	0	3	0
3	B	476	0	0	1	0
All	All	13361	0	12268	141	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 6.

All (141) 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:97:GLU:CD	1:B:327:GLU:HG3	2.07	0.78
1:B:773:LYS:HE2	1:B:777:ASN:HD21	1.47	0.78
1:A:42:THR:O	1:A:50:ARG:HD3	1.84	0.75
1:A:45:GLN:OE1	1:A:49:LEU:HD23	1.91	0.70
1:A:182:ASN:O	1:A:186:GLU:HG3	1.92	0.70
1:A:114:GLU:HG2	3:A:2145:HOH:O	1.91	0.69
1:B:182:ASN:O	1:B:186:GLU:HG3	1.91	0.69
1:A:209:ILE:O	1:A:213:GLU:HG3	1.93	0.69
1:A:718:ASN:HB3	1:A:787:MET:HG2	1.75	0.67
1:A:112:SER:OG	1:A:114:GLU:HG3	1.95	0.67
1:A:466:ASP:O	1:A:469:LYS:HG2	2.00	0.62
1:B:56:LYS:O	1:B:60:GLU:HG3	1.99	0.61
1:A:553:VAL:HG23	3:A:2276:HOH:O	2.01	0.61
1:A:735:GLN:NE2	1:A:760:ARG:HH21	1.99	0.61
1:B:735:GLN:NE2	1:B:760:ARG:HH21	1.99	0.60
1:A:739:ILE:HD13	1:A:744:LEU:HD21	1.83	0.60
1:A:773:LYS:HE2	1:A:777:ASN:HD21	1.66	0.59
1:B:529:CYS:SG	1:B:536:LEU:HD13	2.42	0.59
1:B:552:GLY:O	1:B:556:ILE:HD13	2.03	0.59
1:A:412:ILE:HB	1:A:413:PRO:HD3	1.84	0.58
1:A:30:GLU:HG2	1:A:63:PRO:HG2	1.86	0.58
1:B:381:TRP:CZ2	1:B:383:LYS:HB2	2.39	0.58
1:B:64:ILE:HG23	1:B:222:TYR:CZ	2.40	0.57
1:B:216:ILE:HG23	1:B:253:SER:O	2.04	0.57
1:A:529:CYS:SG	1:A:536:LEU:HD13	2.45	0.57
1:A:2:ILE:HD12	1:A:2:ILE:N	2.20	0.56
1:A:64:ILE:HG23	1:A:222:TYR:CZ	2.41	0.56
1:B:2:ILE:HD12	1:B:2:ILE:N	2.21	0.56
1:A:29:SER:O	1:A:33:ILE:HD13	2.06	0.56
1:B:412:ILE:HB	1:B:413:PRO:HD3	1.86	0.56
1:B:224:LYS:O	1:B:228:GLU:HG3	2.07	0.55
1:A:357:LYS:HG3	1:A:361:MET:HE2	1.89	0.55
1:A:381:TRP:CZ2	1:A:383:LYS:HB2	2.42	0.55
1:A:102:ASN:ND2	1:A:103:LYS:HG3	2.21	0.55
1:A:358:VAL:HA	1:A:361:MET:HE3	1.88	0.55
1:B:357:LYS:HG3	1:B:361:MET:HE2	1.88	0.54
1:A:735:GLN:HE22	1:A:760:ARG:HH21	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:GLU:HG2	1:B:63:PRO:HG2	1.90	0.53
1:B:183:GLU:HG2	1:B:530:ILE:HG21	1.90	0.53
1:A:45:GLN:HG3	1:A:46:PRO:HD2	1.91	0.53
1:A:574:THR:OG1	1:A:577:GLU:HG3	2.09	0.53
1:A:138:TYR:HA	1:B:203:LYS:HE3	1.90	0.52
1:B:209:ILE:O	1:B:213:GLU:HG3	2.09	0.52
1:B:618:LEU:O	1:B:622:ARG:HG3	2.10	0.52
1:B:752:GLU:H	1:B:752:GLU:CD	2.17	0.52
1:A:203:LYS:HE3	1:B:138:TYR:HA	1.92	0.52
1:A:318:LEU:HD13	1:A:374:PRO:HB3	1.90	0.52
1:B:381:TRP:CH2	1:B:383:LYS:HD2	2.45	0.51
1:B:64:ILE:HD12	1:B:222:TYR:CE1	2.45	0.51
1:B:735:GLN:HE22	1:B:760:ARG:HH21	1.58	0.51
1:B:740:ASP:HB3	1:B:743:ILE:HG12	1.92	0.51
1:A:2:ILE:HG22	1:A:3:SER:N	2.26	0.51
1:B:578:LEU:O	1:B:581:THR:HG22	2.12	0.50
1:A:343:ILE:CD1	1:A:379:ARG:HG3	2.42	0.50
1:A:552:GLY:O	1:A:556:ILE:HD13	2.11	0.50
1:A:348:ASN:OD1	1:A:350:GLU:HG2	2.12	0.50
1:A:244:GLU:HA	1:A:244:GLU:OE1	2.12	0.49
1:B:528:ASN:HD22	1:B:528:ASN:N	2.10	0.49
1:A:30:GLU:HG2	1:A:63:PRO:CG	2.43	0.49
1:B:465:PHE:CE2	1:B:468:ASN:HA	2.49	0.48
1:B:466:ASP:O	1:B:469:LYS:HG2	2.12	0.48
1:A:45:GLN:CG	1:A:49:LEU:HB3	2.44	0.48
1:B:343:ILE:CD1	1:B:379:ARG:HG3	2.44	0.48
1:A:343:ILE:HD11	1:A:379:ARG:HG3	1.96	0.48
1:B:739:ILE:HD13	1:B:744:LEU:HD21	1.96	0.47
1:A:216:ILE:HG12	1:A:253:SER:O	2.15	0.47
1:A:336:TYR:N	1:A:337:PRO:CD	2.78	0.47
1:B:713:ASP:O	1:B:717:MET:HG2	2.14	0.47
1:A:718:ASN:HB3	1:A:787:MET:CG	2.44	0.47
1:A:192:ARG:O	1:A:192:ARG:HG3	2.14	0.47
1:A:64:ILE:HD12	1:A:222:TYR:CE1	2.51	0.46
1:B:444:GLY:O	1:B:445:TRP:C	2.58	0.46
1:B:700:LEU:HD11	1:B:763:GLY:N	2.30	0.46
1:A:381:TRP:CH2	1:A:383:LYS:HB2	2.50	0.46
1:B:574:THR:OG1	1:B:577:GLU:HG3	2.14	0.46
1:B:335:GLY:C	1:B:337:PRO:HD3	2.41	0.46
1:A:444:GLY:O	1:A:445:TRP:C	2.58	0.45
1:A:349:SER:HB3	1:A:423:GLU:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:GLU:CD	1:A:352:LYS:HZ3	2.25	0.45
1:B:318:LEU:HD13	1:B:374:PRO:HB3	1.98	0.45
1:A:45:GLN:HG3	1:A:49:LEU:HB3	1.98	0.45
1:A:718:ASN:CB	1:A:787:MET:HG2	2.43	0.45
1:B:387:GLU:CD	1:B:387:GLU:H	2.23	0.45
1:B:377:SER:HB3	1:B:406:TYR:CE1	2.52	0.45
1:B:224:LYS:HE2	1:B:228:GLU:OE2	2.17	0.44
1:B:244:GLU:HA	1:B:244:GLU:OE1	2.17	0.44
1:B:527:ASP:O	1:B:528:ASN:HB2	2.17	0.44
1:A:443:GLU:HA	1:A:443:GLU:OE1	2.17	0.44
1:B:336:TYR:N	1:B:337:PRO:CD	2.80	0.44
1:A:183:GLU:HG2	1:A:530:ILE:HG21	1.99	0.44
1:A:485:ASP:O	1:A:489:LYS:HG3	2.17	0.44
1:A:32:ALA:HB2	1:A:85:VAL:HB	2.00	0.44
1:A:335:GLY:C	1:A:337:PRO:HD3	2.43	0.44
1:A:581:THR:HG23	1:A:589:SER:OG	2.18	0.44
1:A:64:ILE:HG23	1:A:222:TYR:CE2	2.53	0.44
1:A:700:LEU:HD11	1:A:763:GLY:N	2.33	0.44
1:B:443:GLU:HA	1:B:443:GLU:OE1	2.18	0.44
1:A:143:THR:O	1:A:147:VAL:HG23	2.17	0.44
1:A:465:PHE:CE2	1:A:468:ASN:HA	2.52	0.44
1:B:97:GLU:OE1	1:B:327:GLU:HG3	2.17	0.43
1:A:30:GLU:HG2	1:A:63:PRO:CD	2.49	0.43
1:A:489:LYS:HG3	3:A:2254:HOH:O	2.18	0.43
1:A:701:PHE:H	1:A:733:HIS:HD1	1.66	0.43
1:A:729:GLN:O	1:A:730:LYS:HB2	2.19	0.43
1:A:16:LEU:HB2	1:A:316:ILE:HD13	2.00	0.43
1:A:527:ASP:O	1:A:528:ASN:HB2	2.19	0.43
1:B:352:LYS:HD2	3:B:2104:HOH:O	2.18	0.43
1:A:195:ASP:HB3	1:A:198:PHE:HD1	1.84	0.43
1:B:343:ILE:HD11	1:B:379:ARG:HG3	2.01	0.43
1:A:102:ASN:HD22	1:A:102:ASN:N	2.15	0.43
1:A:191:ASN:O	1:A:192:ARG:C	2.61	0.43
1:A:175:VAL:HB	1:A:179:GLY:HA3	2.02	0.42
1:B:187:GLN:HG3	1:B:530:ILE:HG22	2.01	0.42
1:B:191:ASN:O	1:B:192:ARG:C	2.63	0.42
1:A:141:GLU:O	1:A:145:GLU:HG3	2.19	0.42
1:A:350:GLU:HG3	1:A:352:LYS:HG3	2.01	0.42
1:A:465:PHE:CZ	1:A:468:ASN:HA	2.54	0.42
1:A:229:ILE:HG22	1:A:242:LEU:HD13	2.00	0.42
1:B:142:GLU:HG2	1:B:501:HIS:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LYS:O	1:A:60:GLU:HG3	2.20	0.42
1:B:4:LYS:HB2	1:B:391:ARG:NH1	2.35	0.42
1:B:100:ARG:HE	1:B:327:GLU:CD	2.27	0.41
1:A:739:ILE:HG12	1:A:740:ASP:N	2.35	0.41
1:A:349:SER:HB3	1:A:423:GLU:CG	2.50	0.41
1:B:448:SER:O	1:B:449:ALA:HB2	2.20	0.41
1:B:30:GLU:HG2	1:B:63:PRO:CG	2.50	0.41
1:A:284:SER:HA	1:A:285:PRO:HD3	1.85	0.41
1:A:618:LEU:O	1:A:622:ARG:HG3	2.21	0.41
1:B:396:THR:HA	1:B:402:LEU:O	2.21	0.41
1:A:453:LEU:C	1:A:556:ILE:HD11	2.46	0.41
1:A:676:ASP:OD1	1:A:676:ASP:N	2.48	0.41
1:B:597:LYS:HB3	1:B:597:LYS:NZ	2.36	0.41
1:A:195:ASP:HB3	1:A:198:PHE:CD1	2.56	0.41
1:B:32:ALA:HB2	1:B:85:VAL:HB	2.03	0.40
1:B:336:TYR:N	1:B:337:PRO:HD3	2.37	0.40
1:A:726:TYR:CZ	1:A:731:GLY:HA3	2.57	0.40
1:B:12:ARG:HD3	1:B:69:GLN:O	2.22	0.40
1:B:86:PHE:CE1	1:B:279:ASN:HB3	2.57	0.40
1:B:284:SER:HA	1:B:285:PRO:HD3	1.90	0.40
1:A:396:THR:HA	1:A:402:LEU:O	2.21	0.40
1:B:315:TRP:CD1	1:B:374:PRO:HD2	2.57	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	784/787 (100%)	752 (96%)	31 (4%)	1 (0%)	48	34
1	B	784/787 (100%)	751 (96%)	31 (4%)	2 (0%)	36	25
All	All	1568/1574 (100%)	1503 (96%)	62 (4%)	3 (0%)	43	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	641	PRO
1	B	641	PRO
1	B	434	VAL

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	675/676 (100%)	665 (98%)	10 (2%)	57	49
1	B	675/676 (100%)	664 (98%)	11 (2%)	55	47
All	All	1350/1352 (100%)	1329 (98%)	21 (2%)	55	47

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	LEU
1	A	102	ASN
1	A	105	THR
1	A	114	GLU
1	A	202	GLU
1	A	435	GLU
1	A	536	LEU
1	A	641	PRO
1	A	648	PHE
1	A	733	HIS
1	B	12	ARG
1	B	94	LEU
1	B	105	THR
1	B	188	LEU
1	B	202	GLU
1	B	435	GLU
1	B	536	LEU
1	B	641	PRO
1	B	719	LEU
1	B	733	HIS

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Mol	Chain	Res	Type
1	B	752	GLU

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	41	GLN
1	A	102	ASN
1	A	110	GLN
1	A	148	ASN
1	A	382	ASN
1	A	437	GLN
1	A	584	ASN
1	A	588	ASN
1	A	703	GLN
1	A	729	GLN
1	A	735	GLN
1	A	748	GLN
1	A	776	GLN
1	A	777	ASN
1	B	110	GLN
1	B	148	ASN
1	B	206	ASN
1	B	220	ASN
1	B	382	ASN
1	B	437	GLN
1	B	477	ASN
1	B	528	ASN
1	B	584	ASN
1	B	588	ASN
1	B	703	GLN
1	B	729	GLN
1	B	735	GLN
1	B	748	GLN
1	B	776	GLN
1	B	777	ASN

5.3.3 RNA ⓘ

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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	B	1802	-	5,5,5	0.30	0	5,5,5	0.31	0
2	GOL	A	1801	-	5,5,5	0.30	0	5,5,5	0.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	1802	-	-	0/4/4/4	-
2	GOL	A	1801	-	-	0/4/4/4	-

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 [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

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(Å ²)	Q<0.9
1	A	786/787 (99%)	0.66	54 (6%) 23 21	21, 29, 42, 57	0
1	B	786/787 (99%)	0.67	51 (6%) 25 23	19, 30, 43, 57	0
All	All	1572/1574 (99%)	0.66	105 (6%) 24 22	19, 30, 42, 57	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ILE	9.2
1	A	2	ILE	7.7
1	B	149	CYS	5.4
1	A	149	CYS	4.7
1	B	3	SER	4.4
1	A	3	SER	4.3
1	A	752	GLU	4.0
1	A	105	THR	3.8
1	A	297	GLU	3.8
1	A	114	GLU	3.8
1	A	64	ILE	3.6
1	B	588	ASN	3.5
1	B	234	SER	3.4
1	B	4	LYS	3.3
1	B	231	ASP	3.3
1	B	64	ILE	3.3
1	A	192	ARG	3.3
1	B	228	GLU	3.3
1	A	473	PRO	3.3
1	B	192	ARG	3.3
1	A	350	GLU	3.2
1	A	68	ASP	3.2
1	B	105	THR	3.2
1	B	753	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	297	GLU	3.1
1	B	740	ASP	3.0
1	B	752	GLU	3.0
1	A	4	LYS	2.9
1	A	231	ASP	2.9
1	B	227	LYS	2.9
1	B	589	SER	2.9
1	B	504	CYS	2.8
1	A	301	ASN	2.8
1	B	202	GLU	2.8
1	B	230	ALA	2.7
1	A	258	LYS	2.7
1	A	504	CYS	2.7
1	B	739	ILE	2.7
1	B	584	ASN	2.7
1	B	5	GLY	2.6
1	B	320	ASP	2.6
1	A	739	ILE	2.6
1	B	251	LYS	2.6
1	A	253	SER	2.6
1	B	68	ASP	2.6
1	B	496	GLU	2.6
1	A	667	ASP	2.6
1	B	102	ASN	2.5
1	A	228	GLU	2.5
1	B	667	ASP	2.5
1	A	474	LYS	2.5
1	A	482	LYS	2.5
1	B	96	ASP	2.5
1	A	496	GLU	2.4
1	A	300	LYS	2.4
1	A	527	ASP	2.4
1	A	197	ASP	2.4
1	B	585	ASP	2.4
1	B	37	GLU	2.4
1	A	589	SER	2.4
1	B	197	ASP	2.4
1	A	666	ALA	2.4
1	B	590	GLU	2.4
1	A	528	ASN	2.3
1	A	580	LYS	2.3
1	A	121	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	469	LYS	2.3
1	A	489	LYS	2.3
1	B	527	ASP	2.3
1	B	350	GLU	2.3
1	B	581	THR	2.3
1	A	570	GLU	2.3
1	A	756	ASP	2.3
1	A	787	MET	2.3
1	A	565	LYS	2.3
1	A	141	GLU	2.2
1	A	349	SER	2.2
1	B	597	LYS	2.2
1	B	233	THR	2.2
1	B	786	VAL	2.2
1	A	569	ASP	2.2
1	A	251	LYS	2.2
1	A	485	ASP	2.2
1	A	751	PRO	2.2
1	B	186	GLU	2.1
1	B	194	ILE	2.1
1	A	227	LYS	2.1
1	B	482	LYS	2.1
1	B	232	ASN	2.1
1	B	240	ALA	2.1
1	A	728	ASP	2.1
1	B	469	LYS	2.1
1	B	565	LYS	2.1
1	A	202	GLU	2.1
1	A	298	ASN	2.1
1	B	468	ASN	2.1
1	B	710	LEU	2.1
1	B	124	GLU	2.1
1	A	597	LYS	2.0
1	B	245	ILE	2.0
1	A	223	ALA	2.0
1	A	740	ASP	2.0
1	A	741	LYS	2.0
1	A	198	PHE	2.0
1	A	302	ILE	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](#)

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($\text{\AA}^2$)	Q<0.9
2	GOL	B	1802	6/6	0.89	0.12	26,28,29,30	0
2	GOL	A	1801	6/6	0.91	0.11	25,26,28,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.