



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:18 am BST

PDB ID : 4H7N
Title : The Structure of Putative Aldehyde Dehydrogenase PutA from *Anabaena variabilis*.
Authors : Cuff, M.E.; Chhor, G.; Clancy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2012-09-20
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

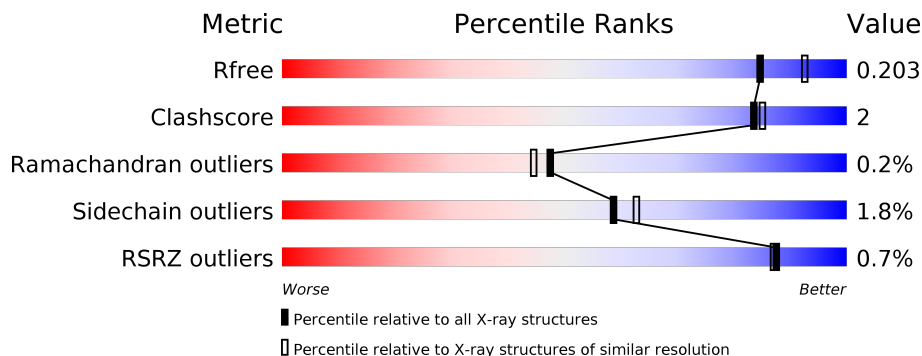
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

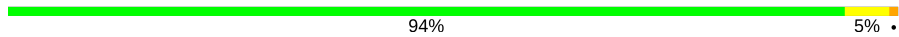
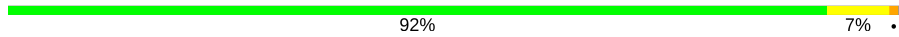


The reported resolution of this entry is 2.00 Å.

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))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 on 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	474	 94% 5% •
1	B	474	 92% 7% ••
1	C	474	 91% 8% •
1	D	474	 2% 91% 7% ••

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 15728 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 Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	472	3623	2317	619	670	7	10	0	1	0
1	B	470	3601	2303	615	667	7	9	0	0	0
1	C	469	3628	2321	622	669	7	9	0	4	0
1	D	468	3585	2295	610	664	7	9	0	1	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q3MAW0
A	-1	ASN	-	EXPRESSION TAG	UNP Q3MAW0
A	0	ALA	-	EXPRESSION TAG	UNP Q3MAW0
B	-2	SER	-	EXPRESSION TAG	UNP Q3MAW0
B	-1	ASN	-	EXPRESSION TAG	UNP Q3MAW0
B	0	ALA	-	EXPRESSION TAG	UNP Q3MAW0
C	-2	SER	-	EXPRESSION TAG	UNP Q3MAW0
C	-1	ASN	-	EXPRESSION TAG	UNP Q3MAW0
C	0	ALA	-	EXPRESSION TAG	UNP Q3MAW0
D	-2	SER	-	EXPRESSION TAG	UNP Q3MAW0
D	-1	ASN	-	EXPRESSION TAG	UNP Q3MAW0
D	0	ALA	-	EXPRESSION TAG	UNP Q3MAW0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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

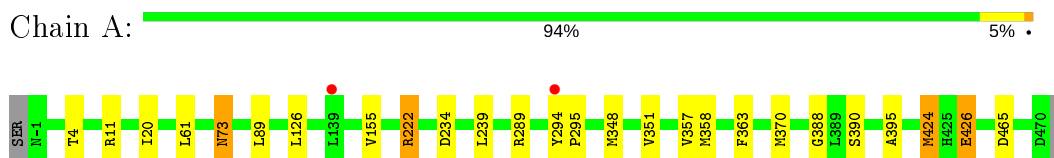
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	322	Total 322	O 322	0	0
3	B	296	Total 296	O 296	0	0
3	C	360	Total 360	O 360	0	0
3	D	223	Total 223	O 223	0	0

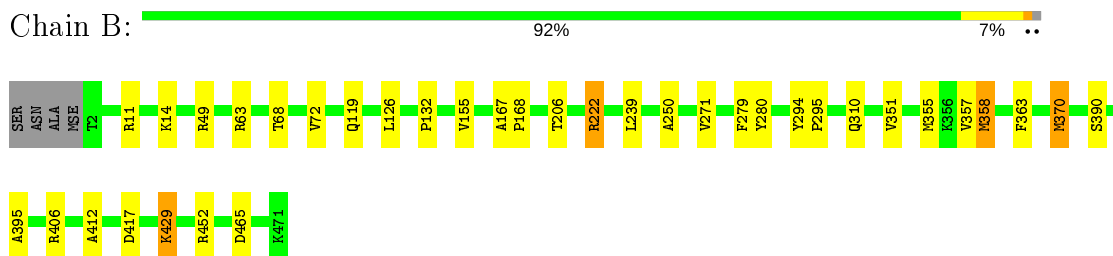
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

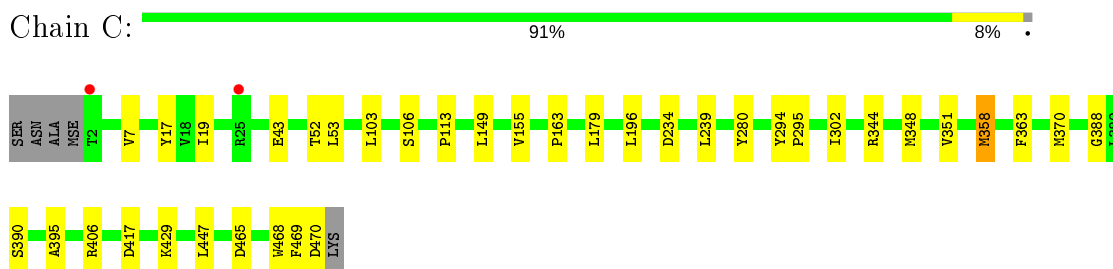
- Molecule 1: Aldehyde dehydrogenase



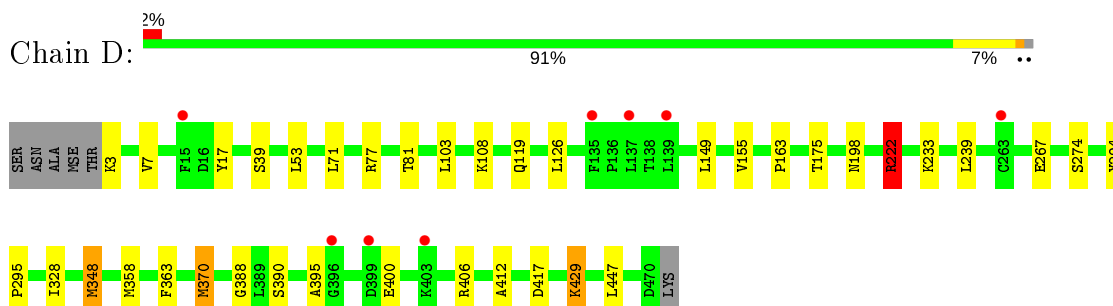
- Molecule 1: Aldehyde dehydrogenase



- Molecule 1: Aldehyde dehydrogenase



- Molecule 1: Aldehyde dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.84Å 88.51Å 123.00Å 90.00° 109.97° 90.00°	Depositor
Resolution (Å)	41.33 – 2.00 41.33 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (41.33-2.00) 99.5 (41.33-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.00Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.156 , 0.196 0.168 , 0.203	Depositor DCC
R_{free} test set	7180 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.1	Xtrriage
Anisotropy	0.407	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15728	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% 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 i

5.1 Standard geometry i

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	0.73	1/3693 (0.0%)	0.85	7/5011 (0.1%)
1	B	0.75	0/3669	0.87	9/4982 (0.2%)
1	C	0.78	0/3708	0.87	4/5032 (0.1%)
1	D	0.71	0/3654	0.81	5/4960 (0.1%)
All	All	0.74	1/14724 (0.0%)	0.85	25/19985 (0.1%)

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	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	426	GLU	CD-OE1	5.63	1.31	1.25

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	222	ARG	NE-CZ-NH2	-9.50	115.55	120.30
1	A	222	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	B	452	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	B	358	MSE	CG-SE-CE	-7.46	82.49	98.90
1	C	358	MSE	CA-CB-CG	-7.39	100.74	113.30
1	B	222	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	D	222	ARG	NE-CZ-NH1	-6.63	116.99	120.30
1	B	406	ARG	NE-CZ-NH2	-6.58	117.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	77	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	11	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	234	ASP	CB-CG-OD1	6.17	123.85	118.30
1	B	11	ARG	NE-CZ-NH2	6.15	123.37	120.30
1	A	222	ARG	CG-CD-NE	-5.86	99.49	111.80
1	B	63	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	11	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	D	222	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	C	234	ASP	CB-CG-OD1	5.53	123.28	118.30
1	B	370	MSE	CG-SE-CE	-5.50	86.79	98.90
1	A	358	MSE	CA-CB-CG	-5.44	104.05	113.30
1	C	406	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	C	370	MSE	CG-SE-CE	-5.29	87.25	98.90
1	B	49	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	D	406	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	424	MSE	CA-CB-CG	-5.09	104.65	113.30
1	D	77	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	3	LYS	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	3623	0	3658	15	0
1	B	3601	0	3624	25	0
1	C	3628	0	3673	17	0
1	D	3585	0	3618	17	0
2	A	24	0	32	0	0
2	B	18	0	24	0	0
2	C	30	0	40	0	0
2	D	18	0	24	0	0
3	A	322	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	296	0	0	3	0
3	C	360	0	0	1	0
3	D	223	0	0	2	0
All	All	15728	0	14693	70	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 2.

All (70) 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:351:VAL:HB	1:B:355:MSE:HE1	1.62	0.80
1:C:344[A]:ARG:NH2	3:C:803:HOH:O	2.21	0.73
1:C:103:LEU:HD21	1:C:447:LEU:HD21	1.76	0.66
1:A:239:LEU:HD12	1:A:395:ALA:HB2	1.83	0.60
1:B:351:VAL:CB	1:B:355:MSE:HE1	2.32	0.59
1:C:239:LEU:HD12	1:C:395:ALA:HB2	1.84	0.59
1:C:19:ILE:HD11	1:C:163:PRO:HG3	1.85	0.59
1:B:355:MSE:HE3	1:B:357:VAL:HG12	1.83	0.58
1:D:103:LEU:HD21	1:D:447:LEU:HD21	1.85	0.58
1:B:355:MSE:HE3	1:B:357:VAL:CG1	2.33	0.58
1:B:355:MSE:HE2	1:B:358:MSE:HG3	1.87	0.57
1:D:126:LEU:HD11	1:D:155:VAL:HG23	1.87	0.56
1:B:412:ALA:HB2	1:B:429:LYS:HD2	1.86	0.56
1:C:351:VAL:HG23	1:C:358:MSE:HE1	1.88	0.55
1:A:348:MSE:HE1	1:A:357:VAL:HG11	1.90	0.53
1:B:417:ASP:OD2	1:C:465:ASP:OD2	2.27	0.53
1:A:289:ARG:NH1	3:A:698:HOH:O	2.42	0.52
1:A:351:VAL:HG23	1:A:370:MSE:HG3	1.92	0.52
1:A:424:MSE:HE2	1:A:426:GLU:OE1	2.08	0.52
1:D:412:ALA:HB2	1:D:429[A]:LYS:HD2	1.92	0.51
1:D:198:ASN:HA	1:D:222:ARG:CD	2.41	0.51
1:B:358:MSE:HE1	1:B:370:MSE:SE	2.60	0.51
1:A:426:GLU:HG2	3:A:786:HOH:O	2.10	0.50
1:A:294:TYR:CD1	1:A:295:PRO:HA	2.46	0.50
1:C:155:VAL:HG11	1:C:196:LEU:HD11	1.93	0.50
1:D:294:TYR:CD1	1:D:295:PRO:HA	2.46	0.50
1:B:126:LEU:HD11	1:B:155:VAL:HG23	1.94	0.49
1:A:465:ASP:OD2	1:D:417:ASP:OD2	2.30	0.49
1:A:4:THR:HG22	1:A:20:ILE:HD12	1.95	0.49
1:B:351:VAL:HB	1:B:355:MSE:CE	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:ALA:HB2	1:C:468:TRP:CZ2	2.48	0.49
1:D:328:ILE:HD12	1:D:348:MSE:HE2	1.96	0.48
1:B:222:ARG:HD2	3:B:845:HOH:O	2.13	0.48
1:A:222:ARG:CZ	1:A:222:ARG:HB3	2.43	0.48
1:B:239:LEU:HD12	1:B:395:ALA:HB2	1.95	0.48
1:C:53:LEU:HD12	1:C:149:LEU:HD21	1.95	0.48
1:A:348:MSE:HE3	1:A:351:VAL:CG1	2.44	0.47
1:A:126:LEU:HD11	1:A:155:VAL:HG23	1.97	0.47
1:B:465:ASP:OD2	1:C:417:ASP:OD2	2.33	0.47
1:D:71:LEU:HD23	1:D:81:THR:HG23	1.97	0.47
1:C:7:VAL:HB	1:C:17:TYR:HB3	1.96	0.47
1:C:302:ILE:HD13	1:C:302:ILE:N	2.30	0.46
1:B:271:VAL:HG21	1:B:279:PHE:CD2	2.50	0.45
1:D:274:SER:C	3:D:782:HOH:O	2.55	0.45
1:B:355:MSE:CE	1:B:358:MSE:HG3	2.47	0.45
1:D:175:THR:HG22	1:D:175:THR:O	2.17	0.45
1:B:132:PRO:HD3	1:B:206:THR:HB	1.98	0.44
1:B:167:ALA:HB3	1:B:168:PRO:CD	2.48	0.44
1:D:7:VAL:HB	1:D:17:TYR:HB3	1.99	0.44
1:C:294:TYR:CD1	1:C:295:PRO:HA	2.52	0.44
1:D:358:MSE:HE1	1:D:370:MSE:SE	2.68	0.43
1:C:351:VAL:CG2	1:C:358:MSE:HE1	2.48	0.43
1:B:351:VAL:CG1	1:B:355:MSE:HE1	2.49	0.43
1:D:429[B]:LYS:NZ	3:D:744:HOH:O	2.36	0.43
1:D:103:LEU:HD21	1:D:447:LEU:CD2	2.49	0.43
1:D:53:LEU:HD12	1:D:149:LEU:HD21	2.01	0.42
1:B:429:LYS:NZ	3:B:863:HOH:O	2.49	0.41
1:B:68:THR:O	1:B:72:VAL:HG23	2.20	0.41
1:D:239:LEU:HD12	1:D:395:ALA:HB2	2.02	0.41
1:B:310:GLN:NE2	3:B:890:HOH:O	2.53	0.41
1:B:167:ALA:HB3	1:B:168:PRO:HD3	2.02	0.41
1:B:294:TYR:CD1	1:B:295:PRO:HA	2.55	0.41
1:A:4:THR:HG22	1:A:20:ILE:CD1	2.51	0.41
1:D:233:LYS:HD2	1:D:267:GLU:OE1	2.21	0.41
1:C:52:THR:CG2	1:C:179:LEU:HB2	2.51	0.41
1:A:73:ASN:CB	3:A:898:HOH:O	2.69	0.41
1:A:61:LEU:HD21	1:A:89:LEU:HD13	2.03	0.41
1:C:469:PHE:O	1:C:470:ASP:C	2.60	0.41
1:C:155:VAL:CG1	1:C:196:LEU:HD11	2.51	0.40
1:B:357:VAL:HG13	1:B:358:MSE:HG2	2.02	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	471/474 (99%)	462 (98%)	8 (2%)	1 (0%)	47	44
1	B	468/474 (99%)	457 (98%)	11 (2%)	0	100	100
1	C	471/474 (99%)	462 (98%)	8 (2%)	1 (0%)	47	44
1	D	467/474 (98%)	456 (98%)	9 (2%)	2 (0%)	34	30
All	All	1877/1896 (99%)	1837 (98%)	36 (2%)	4 (0%)	47	44

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	163	PRO
1	D	388	GLY
1	A	388	GLY
1	C	388	GLY

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	384/376 (102%)	381 (99%)	3 (1%)	81	86
1	B	381/376 (101%)	375 (98%)	6 (2%)	62	67
1	C	386/376 (103%)	378 (98%)	8 (2%)	53	57
1	D	379/376 (101%)	368 (97%)	11 (3%)	42	43
All	All	1530/1504 (102%)	1502 (98%)	28 (2%)	59	63

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	A	363	PHE
1	A	390	SER
1	B	14	LYS
1	B	119	GLN
1	B	280	TYR
1	B	363	PHE
1	B	390	SER
1	B	429	LYS
1	C	43	GLU
1	C	106	SER
1	C	113	PRO
1	C	280	TYR
1	C	348	MSE
1	C	363	PHE
1	C	390	SER
1	C	429	LYS
1	D	39	SER
1	D	108	LYS
1	D	119	GLN
1	D	222	ARG
1	D	348	MSE
1	D	363	PHE
1	D	370	MSE
1	D	390	SER
1	D	400	GLU
1	D	429[A]	LYS
1	D	429[B]	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

15 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	501	-	5,5,5	0.35	0	5,5,5	0.33	0
2	GOL	A	501	-	5,5,5	0.43	0	5,5,5	0.97	0
2	GOL	D	501	-	5,5,5	0.44	0	5,5,5	0.71	0
2	GOL	C	501	-	5,5,5	0.19	0	5,5,5	0.56	0
2	GOL	C	502	-	5,5,5	0.26	0	5,5,5	0.62	0
2	GOL	C	505	-	5,5,5	0.51	0	5,5,5	0.71	0
2	GOL	A	502	-	5,5,5	0.32	0	5,5,5	0.78	0
2	GOL	B	503	-	5,5,5	0.35	0	5,5,5	0.52	0
2	GOL	C	503	-	5,5,5	0.64	0	5,5,5	0.39	0
2	GOL	A	503	-	5,5,5	0.62	0	5,5,5	0.54	0
2	GOL	D	503	-	5,5,5	0.38	0	5,5,5	0.73	0
2	GOL	B	502	-	5,5,5	0.44	0	5,5,5	0.26	0
2	GOL	A	504	-	5,5,5	0.46	0	5,5,5	0.44	0
2	GOL	C	504	-	5,5,5	0.58	0	5,5,5	0.36	0
2	GOL	D	502	-	5,5,5	0.63	0	5,5,5	0.73	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	501	-	-	2/4/4/4	-
2	GOL	A	501	-	-	2/4/4/4	-
2	GOL	D	501	-	-	0/4/4/4	-
2	GOL	C	501	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	C	502	-	-	2/4/4/4	-
2	GOL	C	505	-	-	2/4/4/4	-
2	GOL	A	502	-	-	2/4/4/4	-
2	GOL	B	503	-	-	2/4/4/4	-
2	GOL	C	503	-	-	4/4/4/4	-
2	GOL	A	503	-	-	2/4/4/4	-
2	GOL	D	503	-	-	2/4/4/4	-
2	GOL	B	502	-	-	2/4/4/4	-
2	GOL	A	504	-	-	0/4/4/4	-
2	GOL	C	504	-	-	2/4/4/4	-
2	GOL	D	502	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GOL	O1-C1-C2-C3
2	C	505	GOL	O2-C2-C3-O3
2	A	502	GOL	O1-C1-C2-C3
2	B	503	GOL	O1-C1-C2-O2
2	B	503	GOL	O1-C1-C2-C3
2	C	503	GOL	O1-C1-C2-C3
2	C	503	GOL	C1-C2-C3-O3
2	A	503	GOL	O1-C1-C2-C3
2	D	503	GOL	O1-C1-C2-C3
2	B	502	GOL	C1-C2-C3-O3
2	B	502	GOL	O2-C2-C3-O3
2	D	502	GOL	C1-C2-C3-O3
2	B	501	GOL	O1-C1-C2-C3
2	C	501	GOL	O1-C1-C2-C3
2	C	502	GOL	C1-C2-C3-O3
2	C	505	GOL	C1-C2-C3-O3
2	C	504	GOL	C1-C2-C3-O3
2	D	502	GOL	O1-C1-C2-C3
2	B	501	GOL	O1-C1-C2-O2
2	A	502	GOL	O1-C1-C2-O2
2	C	503	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	C	503	GOL	O2-C2-C3-O3
2	D	503	GOL	O1-C1-C2-O2
2	C	504	GOL	O2-C2-C3-O3
2	D	502	GOL	O2-C2-C3-O3
2	A	501	GOL	O1-C1-C2-O2
2	A	503	GOL	O1-C1-C2-O2
2	D	502	GOL	O1-C1-C2-O2
2	C	502	GOL	O2-C2-C3-O3
2	C	501	GOL	O1-C1-C2-O2
2	C	501	GOL	C1-C2-C3-O3

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 [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	462/474 (97%)	-0.33	2 (0%) 92 92	20, 32, 49, 68	0
1	B	461/474 (97%)	-0.48	0 100 100	20, 34, 53, 63	0
1	C	460/474 (97%)	-0.45	2 (0%) 92 92	18, 29, 50, 76	0
1	D	459/474 (96%)	-0.16	8 (1%) 70 68	21, 36, 57, 73	0
All	All	1842/1896 (97%)	-0.36	12 (0%) 87 87	18, 33, 53, 76	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	THR	4.9
1	D	403	LYS	3.6
1	D	263	CYS	3.1
1	D	15	PHE	2.8
1	C	25	ARG	2.8
1	D	137	LEU	2.6
1	D	139	LEU	2.5
1	A	294	TYR	2.4
1	D	399	ASP	2.3
1	D	396	GLY	2.1
1	A	139	LEU	2.1
1	D	135	PHE	2.1

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 carbohydrates 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(Å ²)	Q<0.9
2	GOL	A	503	6/6	0.70	0.18	57,60,64,67	0
2	GOL	A	504	6/6	0.74	0.29	58,60,64,66	0
2	GOL	C	505	6/6	0.77	0.17	45,50,58,64	0
2	GOL	C	504	6/6	0.78	0.32	64,66,69,75	0
2	GOL	D	503	6/6	0.80	0.18	47,52,58,67	0
2	GOL	B	502	6/6	0.81	0.22	63,73,76,76	0
2	GOL	C	503	6/6	0.84	0.37	57,60,61,62	0
2	GOL	D	502	6/6	0.84	0.30	57,61,62,66	0
2	GOL	A	502	6/6	0.86	0.19	43,56,60,64	0
2	GOL	C	502	6/6	0.89	0.13	38,46,47,52	0
2	GOL	A	501	6/6	0.91	0.30	47,58,59,59	0
2	GOL	B	503	6/6	0.92	0.12	54,58,59,62	0
2	GOL	C	501	6/6	0.93	0.17	52,55,63,72	0
2	GOL	B	501	6/6	0.94	0.09	36,42,49,52	0
2	GOL	D	501	6/6	0.95	0.12	42,47,54,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.