



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 05:18 AM UTC

PDB ID : 4KCA / pdb_00004kca
Title : Crystal Structure of Endo-1,5-alpha-L-arabinanase from a Bovine Ruminant Metagenomic Library
Authors : Santos, C.R.; Polo, C.C.; Costa, M.C.M.F.; Nascimento, A.F.Z.; Wong, D.W.S.; Murakami, M.T.
Deposited on : 2013-04-24
Resolution : 1.90 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

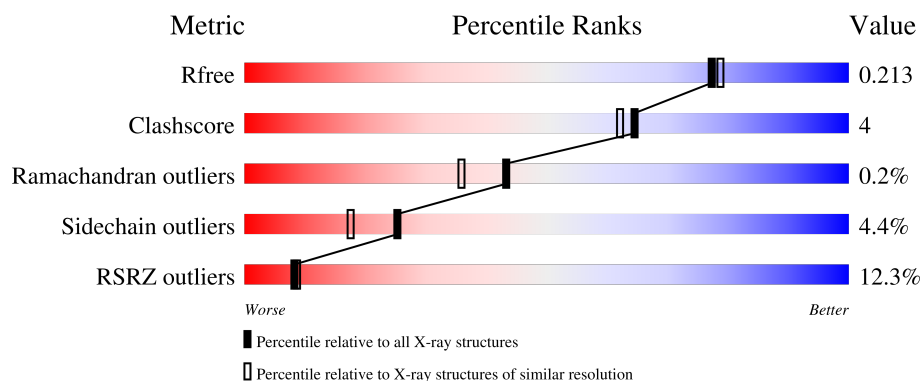
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	692	11% 83% 7% 8%
1	B	692	12% 82% 9% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IOD	A	725	-	-	X	-
2	IOD	A	730	-	-	X	-
2	IOD	B	712	-	-	X	-
2	IOD	B	726	-	-	X	-
2	IOD	B	727	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10809 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.

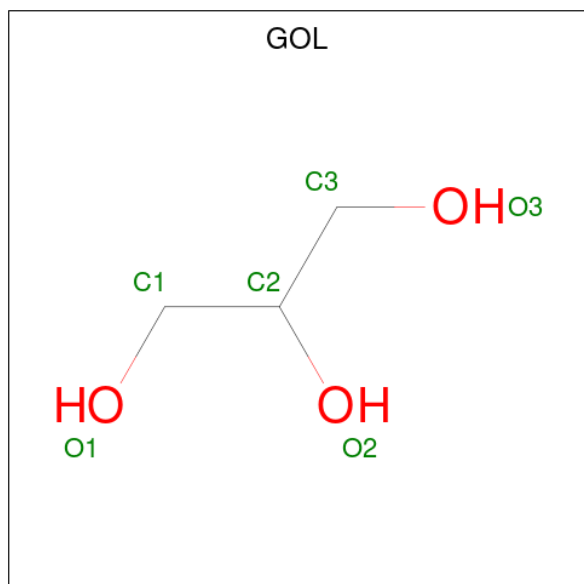
- Molecule 1 is a protein called Endo-1,5-alpha-L-arabinanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	635	Total	C	N	O	S	0	1	0
			4941	3160	812	958	11			
1	B	637	Total	C	N	O	S	0	1	0
			4956	3168	814	963	11			

- Molecule 2 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	33	Total	I	0	0
			33	33		
2	B	30	Total	I	0	0
			30	30		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	B	1	Total	Na	0	0
			1	1		

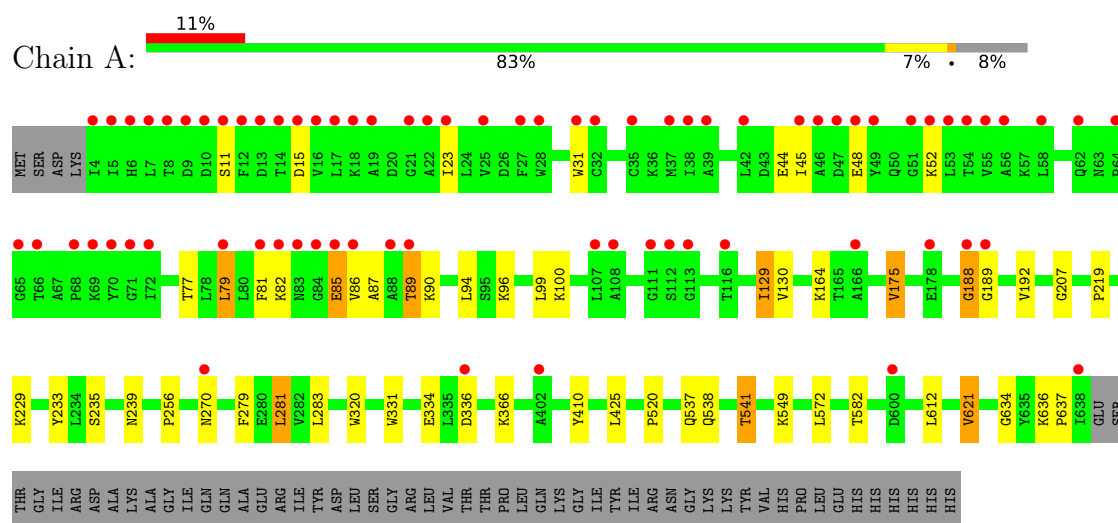
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	420	Total	O	0	0
			420	420		
5	B	415	Total	O	0	0
			415	415		

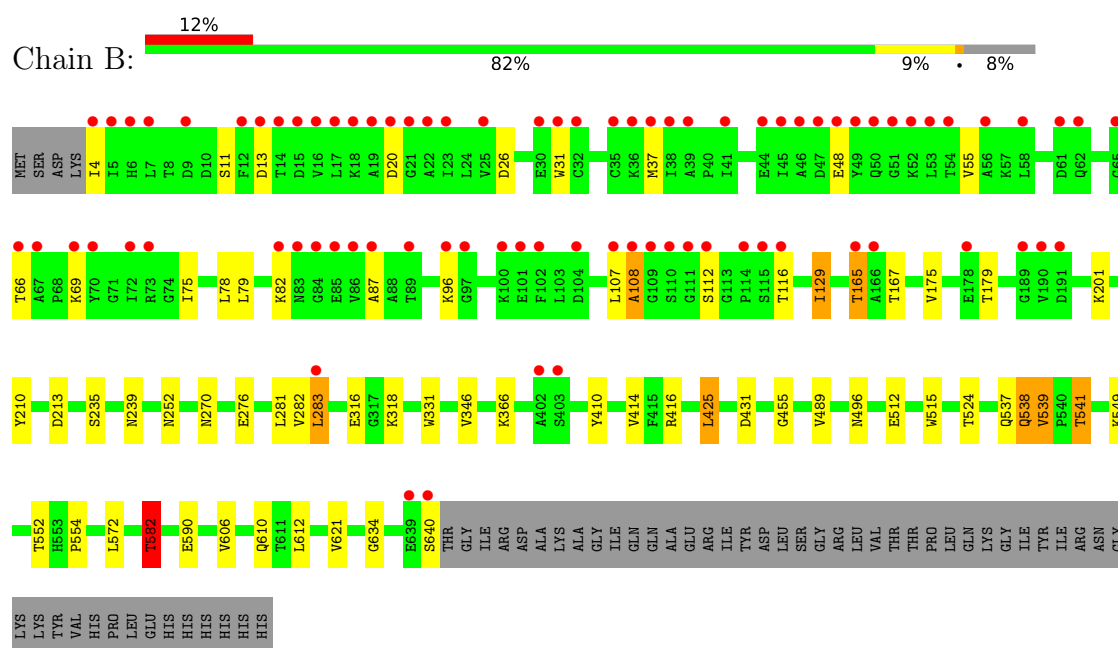
3 Residue-property plots

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: Endo-1,5-alpha-L-arabinanase



• Molecule 1: Endo-1,5-alpha-L-arabinanase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.91Å 114.32Å 167.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.84 – 1.90 41.84 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.2 (41.84-1.90) 98.2 (41.84-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.187 , 0.216 0.183 , 0.213	Depositor DCC
R_{free} test set	7535 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.527	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10809	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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

Bond lengths and bond angles in the following residue types are not validated in this section: IOD, NA, 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	0.93	0/5078	0.99	3/6907 (0.0%)
1	B	0.91	2/5093 (0.0%)	0.97	5/6927 (0.1%)
All	All	0.92	2/10171 (0.0%)	0.98	8/13834 (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	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	455	GLY	N-CA	6.85	1.50	1.44
1	B	179	THR	C-O	-5.41	1.20	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	539	VAL	CB-CA-C	6.70	117.96	110.52
1	B	75	ILE	N-CA-C	5.75	114.22	107.84
1	A	538	GLN	N-CA-C	5.74	117.54	111.28
1	B	582	THR	CB-CA-C	-5.45	98.56	111.65
1	B	213	ASP	N-CA-C	5.42	117.19	111.28
1	A	188	GLY	N-CA-C	5.27	124.71	114.16
1	B	210	TYR	N-CA-C	5.20	117.57	110.24
1	A	175	VAL	N-CA-CB	-5.05	106.32	112.33

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	188	GLY	Peptide

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	4941	0	4742	35	0
1	B	4956	0	4753	31	0
2	A	33	0	0	7	0
2	B	30	0	0	9	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	420	0	0	4	0
5	B	415	0	0	7	0
All	All	10809	0	9511	75	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 4.

All (75) 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:537:GLN:HE22	1:A:541:THR:HG22	1.04	1.11
2:B:717:IOD:I	2:B:729:IOD:I	3.11	1.09
2:A:721:IOD:I	2:B:725:IOD:I	3.16	1.02
1:B:537:GLN:HE22	1:B:541:THR:HG22	1.19	1.02
1:B:496:ASN:ND2	2:B:727:IOD:I	2.66	0.97
1:A:537:GLN:NE2	1:A:541:THR:HG22	1.81	0.95
2:B:719:IOD:I	2:B:726:IOD:I	3.43	0.77
1:A:192:VAL:HG21	1:A:281:LEU:HD21	1.66	0.77
1:A:537:GLN:HE22	1:A:541:THR:CG2	1.93	0.76
2:A:731:IOD:I	2:A:733:IOD:I	3.45	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:VAL:CG2	1:A:281:LEU:HD21	2.20	0.71
1:A:23:ILE:HG23	1:A:81:PHE:HB2	1.73	0.70
1:B:512:GLU:HG3	5:B:834:HOH:O	1.92	0.70
2:A:720:IOD:I	2:A:732:IOD:I	3.50	0.69
1:A:164:LYS:HB2	1:A:256:PRO:HB2	1.77	0.67
1:A:48:GLU:HG2	1:A:100:LYS:NZ	2.10	0.65
1:A:90:LYS:HG2	1:A:94:LEU:HD11	1.79	0.64
1:B:537:GLN:NE2	1:B:541:THR:HG22	2.02	0.64
1:B:270:ASN:ND2	5:B:1057:HOH:O	2.09	0.63
1:A:23:ILE:CG2	1:A:81:PHE:HB2	2.29	0.63
1:B:252[A]:ASN:ND2	5:B:1191:HOH:O	2.13	0.63
1:A:270:ASN:ND2	5:A:1067:HOH:O	2.02	0.63
1:A:79:LEU:HD12	1:A:89:THR:HB	1.86	0.57
1:B:165:THR:HG22	1:B:167:THR:H	1.69	0.57
1:B:129:ILE:HD13	1:B:489:VAL:HG21	1.89	0.55
1:B:276:GLU:HG3	5:B:1210:HOH:O	2.06	0.55
2:B:714:IOD:I	2:B:722:IOD:I	3.65	0.55
1:A:229:LYS:NZ	2:A:730:IOD:I	3.10	0.55
2:A:730:IOD:I	5:A:1161:HOH:O	2.89	0.54
1:B:239:ASN:ND2	2:B:711:IOD:I	3.11	0.54
1:B:610:GLN:HG3	1:B:621:VAL:HG21	1.90	0.53
1:A:82:LYS:HD2	1:A:87:ALA:HB2	1.90	0.53
1:A:239:ASN:ND2	2:A:725:IOD:I	3.12	0.53
1:A:82:LYS:HD2	1:A:87:ALA:CB	2.39	0.52
1:B:538:GLN:HG3	5:B:824:HOH:O	2.11	0.50
1:A:192:VAL:HG21	1:A:281:LEU:CD2	2.39	0.50
1:B:582:THR:HG21	5:B:1166:HOH:O	2.11	0.50
1:A:520:PRO:HG2	1:A:621:VAL:HG23	1.94	0.49
1:B:549:LYS:O	1:B:634:GLY:HA2	2.13	0.49
2:B:712:IOD:I	5:B:1203:HOH:O	2.91	0.48
1:A:85:GLU:HG3	1:A:86:VAL:H	1.79	0.47
1:A:45:ILE:HG13	1:A:99:LEU:HD23	1.96	0.46
1:A:77:THR:HG22	1:A:79:LEU:HD13	1.98	0.46
1:A:48:GLU:HG2	1:A:100:LYS:HZ1	1.81	0.46
1:B:541:THR:HG21	1:B:590:GLU:CD	2.40	0.46
1:A:44:GLU:OE1	1:A:96:LYS:NZ	2.41	0.46
1:B:4:ILE:HA	1:B:55:VAL:O	2.16	0.45
2:B:726:IOD:I	2:B:727:IOD:I	3.74	0.45
1:B:107:LEU:O	1:B:108:ALA:HB2	2.15	0.45
1:B:282:VAL:HG12	1:B:283:LEU:HD23	1.97	0.44
1:A:219:PRO:HA	1:A:233:TYR:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ILE:HG13	1:A:130:VAL:N	2.32	0.43
1:B:416:ARG:HG2	1:B:515:TRP:CH2	2.54	0.43
1:A:207:GLY:HA3	2:A:725:IOD:I	2.89	0.43
1:B:66:THR:HA	1:B:69:LYS:HE2	1.99	0.43
1:B:107:LEU:O	1:B:108:ALA:CB	2.67	0.42
1:A:189:GLY:HA2	5:A:1107:HOH:O	2.19	0.42
1:B:26:ASP:HB2	1:B:78:LEU:CD2	2.49	0.42
1:B:201:LYS:HD3	2:B:712:IOD:I	2.89	0.42
1:A:331:TRP:CZ2	1:A:366:LYS:HE2	2.55	0.42
1:B:425:LEU:HD12	1:B:431:ASP:HA	2.00	0.42
1:A:549:LYS:HE3	5:A:845:HOH:O	2.18	0.42
1:A:549:LYS:O	1:A:634:GLY:HA2	2.20	0.42
1:A:192:VAL:HG23	1:A:281:LEU:HD21	1.99	0.42
1:B:541:THR:HG21	1:B:590:GLU:OE2	2.21	0.41
1:B:610:GLN:CG	1:B:621:VAL:HG21	2.49	0.41
1:B:621:VAL:O	1:B:621:VAL:HG23	2.20	0.41
1:A:279:PHE:CZ	1:A:283:LEU:HD12	2.55	0.41
1:A:320:TRP:CZ3	1:A:334:GLU:HG2	2.55	0.41
1:A:11:SER:O	1:A:15:ASP:HB2	2.20	0.41
1:B:331:TRP:CZ2	1:B:366:LYS:HE2	2.56	0.41
1:B:552:THR:O	1:B:554:PRO:HD3	2.21	0.41
1:B:82:LYS:HE2	1:B:87:ALA:CB	2.51	0.40
1:B:318:LYS:HB3	1:B:318:LYS:HE2	1.81	0.40
1:A:636:LYS:HG2	1:A:637:PRO:O	2.21	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	634/692 (92%)	619 (98%)	15 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	636/692 (92%)	617 (97%)	16 (2%)	3 (0%)	24	16
All	All	1270/1384 (92%)	1236 (97%)	31 (2%)	3 (0%)	43	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	108	ALA
1	B	112	SER
1	B	11	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	516/564 (92%)	499 (97%)	17 (3%)	33	26
1	B	518/564 (92%)	490 (95%)	28 (5%)	20	12
All	All	1034/1128 (92%)	989 (96%)	45 (4%)	25	17

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	TRP
1	A	52	LYS
1	A	79	LEU
1	A	85	GLU
1	A	89	THR
1	A	129	ILE
1	A	175	VAL
1	A	235	SER
1	A	281	LEU
1	A	336	ASP
1	A	410	TYR
1	A	425	LEU
1	A	541	THR

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Mol	Chain	Res	Type
1	A	572	LEU
1	A	582	THR
1	A	612	LEU
1	A	621	VAL
1	B	13	ASP
1	B	20	ASP
1	B	31	TRP
1	B	37	MET
1	B	48	GLU
1	B	79	LEU
1	B	96	LYS
1	B	116	THR
1	B	129	ILE
1	B	165	THR
1	B	175	VAL
1	B	235	SER
1	B	281	LEU
1	B	283	LEU
1	B	316	GLU
1	B	346	VAL
1	B	410	TYR
1	B	414	VAL
1	B	425	LEU
1	B	524	THR
1	B	538	GLN
1	B	539	VAL
1	B	541	THR
1	B	572	LEU
1	B	582	THR
1	B	606	VAL
1	B	612	LEU
1	B	640	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	448	ASN
1	A	573	ASN
1	B	106	ASN
1	B	260	GLN
1	B	496	ASN
1	B	573	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 ⓘ

Of 67 ligands modelled in this entry, 65 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
3	GOL	A	734	-	5,5,5	0.53	0	5,5,5	0.92	0
3	GOL	B	731	-	5,5,5	0.42	0	5,5,5	0.69	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
3	GOL	A	734	-	-	2/4/4/4	-
3	GOL	B	731	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	734	GOL	O1-C1-C2-C3
3	A	734	GOL	O1-C1-C2-O2

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	635/692 (91%)	0.37	74 (11%)  	17, 27, 60, 105	6 (0%)
1	B	637/692 (92%)	0.41	82 (12%)  	18, 28, 72, 105	6 (0%)
All	All	1272/1384 (91%)	0.39	156 (12%)  	17, 27, 65, 105	12 (0%)

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	16	VAL	6.2
1	A	17	LEU	6.2
1	B	108	ALA	6.0
1	B	19	ALA	5.8
1	B	112	SER	5.7
1	A	5	ILE	5.6
1	A	6	HIS	5.5
1	B	22	ALA	5.4
1	A	12	PHE	5.4
1	A	25	VAL	5.2
1	B	21	GLY	5.1
1	A	66	THR	4.6
1	A	31	TRP	4.6
1	B	31	TRP	4.6
1	A	21	GLY	4.6
1	A	13	ASP	4.4
1	A	4	ILE	4.4
1	A	54	THR	4.4
1	A	19	ALA	4.4
1	A	112	SER	4.3
1	A	47	ASP	4.3
1	A	65	GLY	4.3
1	A	23	ILE	4.2
1	A	600	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	638	ILE	4.1
1	A	11	SER	4.1
1	A	18	LYS	4.1
1	B	35	CYS	4.1
1	B	37	MET	4.0
1	A	22	ALA	4.0
1	B	639	GLU	4.0
1	B	107	LEU	4.0
1	B	111	GLY	4.0
1	A	27	PHE	4.0
1	B	51	GLY	3.9
1	B	109	GLY	3.9
1	A	9	ASP	3.9
1	B	16	VAL	3.9
1	A	37	MET	3.9
1	B	110	SER	3.9
1	A	51	GLY	3.9
1	A	83	ASN	3.8
1	A	48	GLU	3.8
1	B	54	THR	3.8
1	B	402	ALA	3.7
1	B	6	HIS	3.7
1	B	12	PHE	3.7
1	B	18	LYS	3.6
1	A	84	GLY	3.6
1	B	4	ILE	3.6
1	B	7	LEU	3.6
1	A	70	TYR	3.5
1	A	113	GLY	3.5
1	B	23	ILE	3.5
1	A	81	PHE	3.5
1	A	111	GLY	3.5
1	B	66	THR	3.4
1	B	190	VAL	3.4
1	B	116	THR	3.3
1	B	14	THR	3.3
1	A	86	VAL	3.3
1	B	15	ASP	3.2
1	B	20	ASP	3.2
1	A	7	LEU	3.2
1	A	64	PRO	3.2
1	A	38	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	46	ALA	3.2
1	A	68	PRO	3.2
1	A	72	ILE	3.2
1	B	9	ASP	3.2
1	A	8	THR	3.1
1	A	62	GLN	3.1
1	B	17	LEU	3.1
1	B	48	GLU	3.1
1	B	50	GLN	3.1
1	B	41	ILE	3.0
1	B	403	SER	3.0
1	B	32	CYS	3.0
1	A	14	THR	3.0
1	A	42	LEU	2.9
1	B	283	LEU	2.9
1	B	25	VAL	2.9
1	B	86	VAL	2.9
1	A	71	GLY	2.9
1	B	39	ALA	2.9
1	A	35	CYS	2.9
1	B	69	LYS	2.9
1	A	58	LEU	2.8
1	A	53	LEU	2.8
1	A	52	LYS	2.8
1	B	47	ASP	2.8
1	B	85	GLU	2.8
1	B	70	TYR	2.7
1	B	52	LYS	2.7
1	B	38	ILE	2.7
1	A	32	CYS	2.7
1	A	108	ALA	2.7
1	B	56	ALA	2.7
1	B	102	PHE	2.6
1	A	82	LYS	2.6
1	B	5	ILE	2.6
1	B	67	ALA	2.6
1	B	62	GLN	2.6
1	B	114	PRO	2.6
1	B	104	ASP	2.5
1	B	82	LYS	2.5
1	B	97	GLY	2.5
1	A	166	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	85	GLU	2.5
1	B	89	THR	2.5
1	A	15	ASP	2.5
1	B	73	ARG	2.4
1	B	44	GLU	2.4
1	B	640	SER	2.4
1	B	87	ALA	2.4
1	B	96	LYS	2.4
1	A	189	GLY	2.4
1	B	101	GLU	2.4
1	B	46	ALA	2.4
1	B	49	TYR	2.4
1	A	10	ASP	2.4
1	B	72	ILE	2.4
1	A	402	ALA	2.4
1	A	89	THR	2.3
1	A	116	THR	2.3
1	A	178	GLU	2.3
1	B	30	GLU	2.3
1	A	45	ILE	2.3
1	B	83	ASN	2.3
1	B	65	GLY	2.3
1	B	191	ASP	2.3
1	B	178	GLU	2.3
1	A	79	LEU	2.3
1	A	49	TYR	2.3
1	B	84	GLY	2.3
1	B	36	LYS	2.3
1	A	69	LYS	2.3
1	A	56	ALA	2.2
1	B	61	ASP	2.2
1	B	13	ASP	2.2
1	B	115	SER	2.2
1	B	45	ILE	2.2
1	A	270	ASN	2.2
1	A	107	LEU	2.2
1	B	189	GLY	2.1
1	B	53	LEU	2.1
1	A	188	GLY	2.1
1	A	88	ALA	2.1
1	A	28	TRP	2.1
1	A	55	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	39	ALA	2.1
1	A	336	ASP	2.1
1	B	100	LYS	2.0
1	B	165	THR	2.0
1	B	58	LEU	2.0
1	B	166	ALA	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(Å ²)	Q<0.9
2	IOD	A	733	1/1	0.84	0.32	132,132,132,132	0
2	IOD	B	721	1/1	0.86	0.27	131,131,131,131	0
2	IOD	B	718	1/1	0.87	0.22	91,91,91,91	0
4	NA	A	735	1/1	0.87	0.10	41,41,41,41	0
2	IOD	A	723	1/1	0.88	0.29	82,82,82,82	0
2	IOD	B	722	1/1	0.88	0.23	101,101,101,101	0
2	IOD	B	730	1/1	0.88	0.25	122,122,122,122	0
2	IOD	A	732	1/1	0.88	0.29	98,98,98,98	0
3	GOL	B	731	6/6	0.89	0.13	37,44,45,47	0
2	IOD	B	728	1/1	0.90	0.24	89,89,89,89	0
2	IOD	A	731	1/1	0.91	0.34	92,92,92,92	0
3	GOL	A	734	6/6	0.93	0.12	37,45,47,50	0
2	IOD	A	726	1/1	0.93	0.18	108,108,108,108	0
2	IOD	A	728	1/1	0.93	0.30	87,87,87,87	0
2	IOD	B	723	1/1	0.94	0.24	98,98,98,98	0
2	IOD	B	717	1/1	0.94	0.24	79,79,79,79	0
2	IOD	B	715	1/1	0.94	0.15	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	IOD	B	729	1/1	0.95	0.27	88,88,88,88	0
2	IOD	B	702	1/1	0.95	0.20	108,108,108,108	0
2	IOD	A	721	1/1	0.95	0.25	74,74,74,74	0
2	IOD	A	705	1/1	0.95	0.24	77,77,77,77	0
2	IOD	A	730	1/1	0.95	0.36	92,92,92,92	0
4	NA	B	732	1/1	0.95	0.11	40,40,40,40	0
2	IOD	B	724	1/1	0.96	0.29	80,80,80,80	0
2	IOD	B	711	1/1	0.96	0.33	78,78,78,78	0
2	IOD	A	719	1/1	0.96	0.17	63,63,63,63	0
2	IOD	A	704	1/1	0.96	0.33	99,99,99,99	0
2	IOD	A	722	1/1	0.96	0.24	71,71,71,71	0
2	IOD	A	712	1/1	0.96	0.20	54,54,54,54	0
2	IOD	A	724	1/1	0.96	0.15	90,90,90,90	0
2	IOD	A	715	1/1	0.96	0.07	39,39,39,39	0
2	IOD	A	710	1/1	0.97	0.19	58,58,58,58	0
2	IOD	A	725	1/1	0.97	0.31	73,73,73,73	0
2	IOD	B	701	1/1	0.97	0.32	82,82,82,82	0
2	IOD	A	720	1/1	0.97	0.18	61,61,61,61	0
2	IOD	B	725	1/1	0.97	0.37	81,81,81,81	0
2	IOD	B	726	1/1	0.97	0.38	94,94,94,94	0
2	IOD	B	727	1/1	0.97	0.33	87,87,87,87	0
2	IOD	B	706	1/1	0.97	0.23	70,70,70,70	0
2	IOD	A	703	1/1	0.97	0.34	80,80,80,80	0
2	IOD	A	729	1/1	0.97	0.28	83,83,83,83	0
2	IOD	B	716	1/1	0.97	0.22	67,67,67,67	0
2	IOD	A	708	1/1	0.97	0.24	86,86,86,86	0
2	IOD	A	718	1/1	0.97	0.15	61,61,61,61	0
2	IOD	B	720	1/1	0.97	0.26	72,72,72,72	0
2	IOD	A	709	1/1	0.98	0.22	57,57,57,57	0
2	IOD	A	707	1/1	0.98	0.28	64,64,64,64	0
2	IOD	B	719	1/1	0.98	0.22	64,64,64,64	0
2	IOD	B	703	1/1	0.98	0.31	62,62,62,62	0
2	IOD	A	711	1/1	0.98	0.24	74,74,74,74	0
2	IOD	A	706	1/1	0.98	0.29	72,72,72,72	0
2	IOD	B	713	1/1	0.98	0.30	74,74,74,74	0
2	IOD	A	713	1/1	0.98	0.17	67,67,67,67	0
2	IOD	A	727	1/1	0.98	0.27	80,80,80,80	0
2	IOD	A	701	1/1	0.99	0.04	35,35,35,35	0
2	IOD	B	712	1/1	0.99	0.13	45,45,45,45	0
2	IOD	A	714	1/1	0.99	0.20	55,55,55,55	0
2	IOD	B	714	1/1	0.99	0.15	55,55,55,55	0
2	IOD	A	702	1/1	0.99	0.14	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	IOD	B	704	1/1	0.99	0.18	52,52,52,52	0
2	IOD	B	705	1/1	0.99	0.20	60,60,60,60	0
2	IOD	A	716	1/1	0.99	0.10	44,44,44,44	0
2	IOD	B	707	1/1	0.99	0.27	65,65,65,65	0
2	IOD	B	708	1/1	0.99	0.02	35,35,35,35	0
2	IOD	B	709	1/1	0.99	0.22	62,62,62,62	0
2	IOD	B	710	1/1	0.99	0.05	38,38,38,38	0
2	IOD	A	717	1/1	1.00	0.11	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.