



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 28, 2019 – 01:39 PM EDT

PDB ID : 1CB8
Title : CHONDROITINASE AC LYASE FROM FLAVOBACTERIUM HEPARINUM
Authors : Fethiere, J.; Eggimann, B.; Cygler, M.
Deposited on : 1999-03-02
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

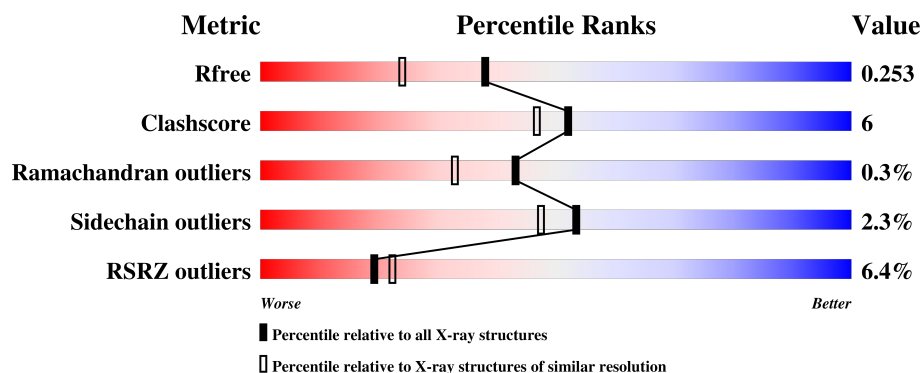
1 Overall quality at a glance

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}	111664	5502 (1.90-1.90)
Clashscore	122126	6115 (1.90-1.90)
Ramachandran outliers	120053	6048 (1.90-1.90)
Sidechain outliers	120020	6048 (1.90-1.90)
RSRZ outliers	108989	5379 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	678	<div> <div>6%</div> <div>85%</div> <div>14%</div> </div>

2 Entry composition [i](#)

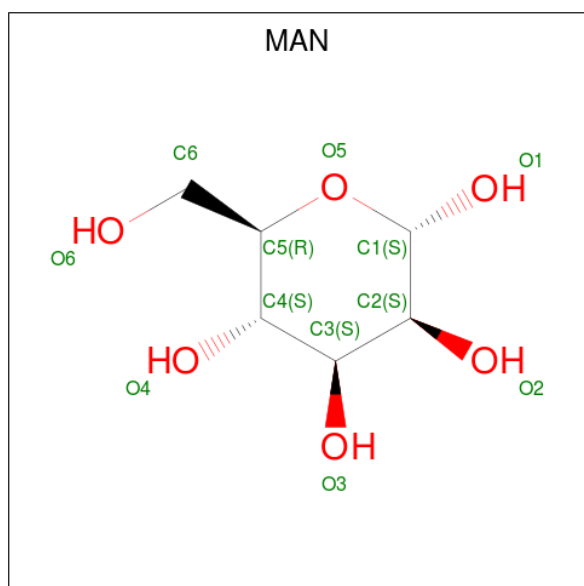
There are 9 unique types of molecules in this entry. The entry contains 5969 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (CHONDROITINASE AC).

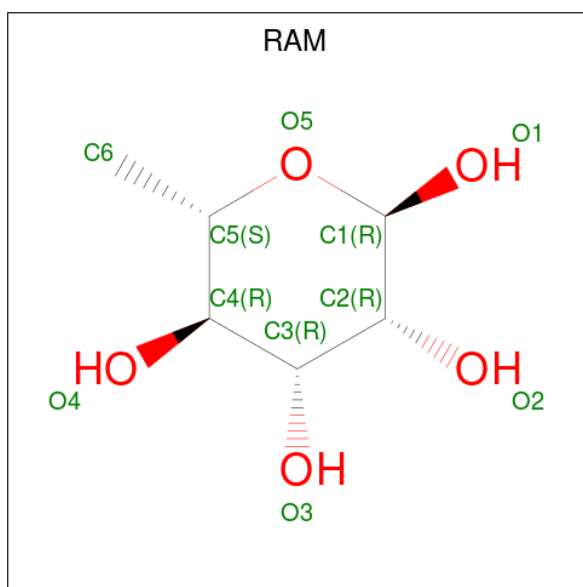
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	675	5383	3445	920	1004	14	98	0	1

- Molecule 2 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



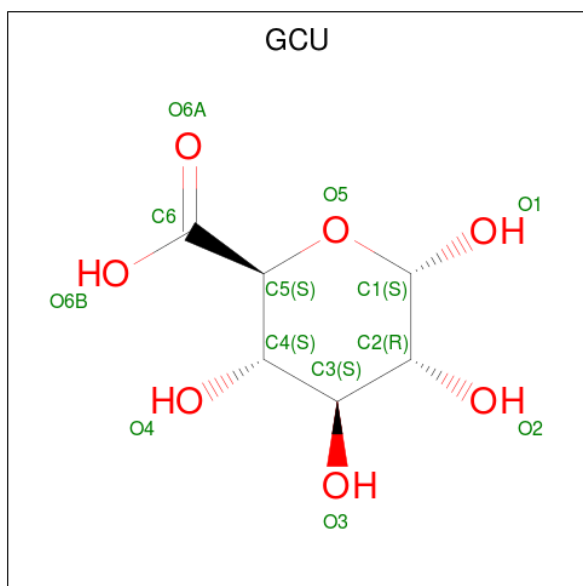
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	11	6	5	0	0

- Molecule 3 is ALPHA-L-RHAMNOSE (three-letter code: RAM) (formula: C₆H₁₂O₅).



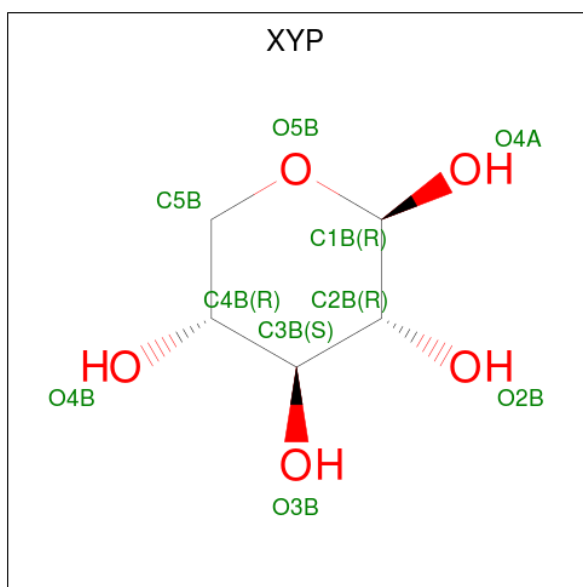
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is D-GLUCURONIC ACID (three-letter code: GCU) (formula: $C_6H_{10}O_7$).



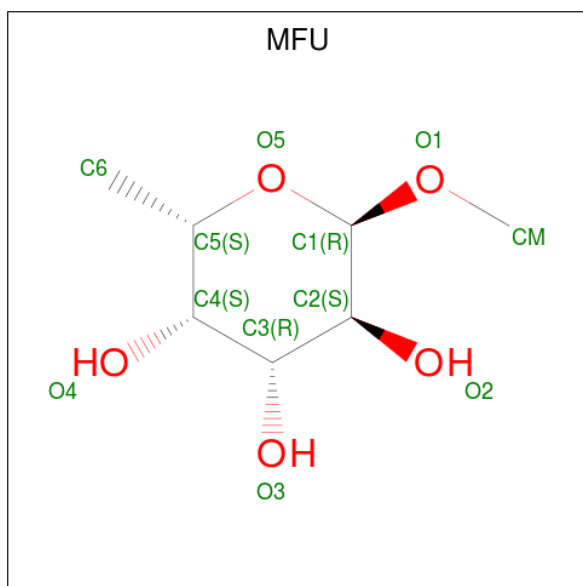
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 5 is BETA-D-XYLOPYRANOSE (three-letter code: XYP) (formula: $C_5H_{10}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			9	5	4		

- Molecule 6 is ALPHA-L-METHYL-FUCOSE (three-letter code: MFU) (formula: $C_7H_{14}O_5$).

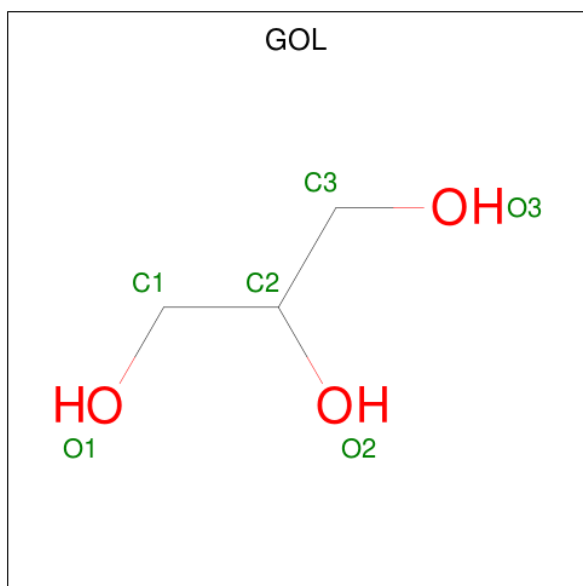


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	11	0
			11	7	4		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

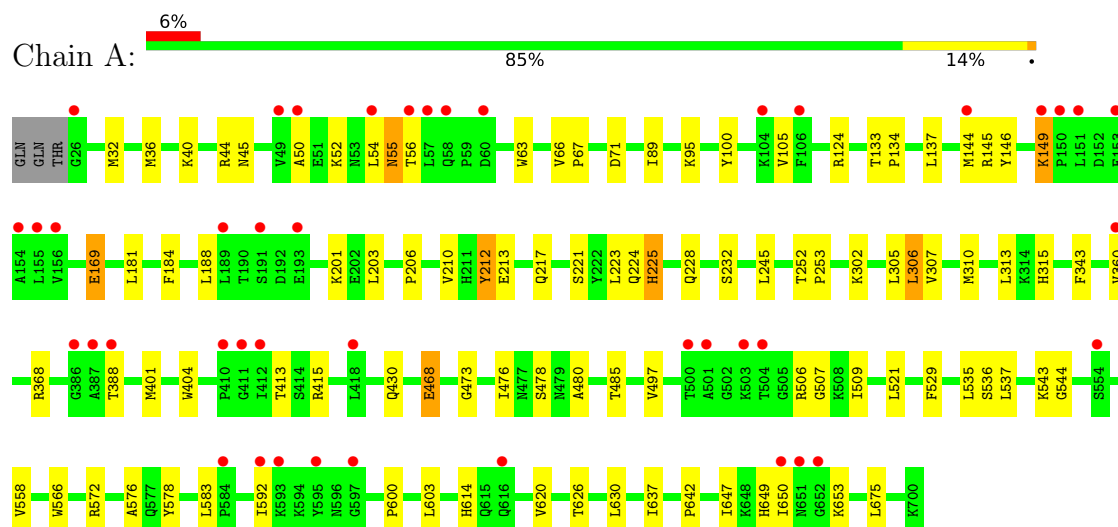
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	526	Total	O	0	0
			526	526		

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: PROTEIN (CHONDROITINASE AC)



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	87.20Å 87.20Å 193.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 1.90 33.36 – 1.83	Depositor EDS
% Data completeness (in resolution range)	92.2 (6.00-1.90) 91.0 (33.36-1.83)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.27 (at 1.83Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.195 , 0.260 0.200 , 0.253	Depositor DCC
R_{free} test set	6133 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 71.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5969	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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: XYP, GOL, CA, RAM, GCU, MFU, MAN

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	0.43	0/5521	0.68	1/7489 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	SER	N-CA-C	-5.59	95.91	111.00

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	5383	0	5241	60	0
2	A	11	0	8	2	0
3	A	10	0	10	2	0
4	A	12	0	6	1	0
5	A	9	0	7	0	0
6	A	11	0	9	0	0
7	A	1	0	0	0	0
8	A	6	0	8	0	0
9	A	526	0	0	3	0
All	All	5969	0	5289	62	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 (62) 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:89:ILE:HG23	1:A:144:MET:HE3	1.57	0.84
1:A:32:MET:HE2	1:A:188:LEU:HB3	1.75	0.68
1:A:89:ILE:HG23	1:A:144:MET:CE	2.24	0.67
1:A:212:TYR:H	1:A:217:GLN:HE22	1.44	0.65
1:A:468:GLU:HB3	1:A:583:LEU:HD23	1.79	0.65
1:A:56:THR:HG23	1:A:63:TRP:CD1	2.34	0.62
1:A:144:MET:SD	9:A:3516:HOH:O	2.55	0.60
1:A:415:ARG:HH22	4:A:2002:GCU:C6	2.14	0.60
1:A:603:LEU:HD13	1:A:630:LEU:HD11	1.84	0.60
1:A:210:VAL:HB	1:A:213:GLU:CG	2.33	0.58
2:A:2000:MAN:H61	3:A:2001:RAM:H2	1.86	0.58
1:A:368:ARG:NH1	1:A:430:GLN:HG3	2.20	0.57
1:A:620:VAL:HG23	1:A:650:ILE:HG21	1.86	0.56
1:A:473:GLY:HA3	1:A:578:TYR:CE2	2.41	0.55
1:A:181:LEU:O	1:A:184:PHE:HB3	2.07	0.55
1:A:368:ARG:HD3	1:A:430:GLN:HA	1.87	0.55
1:A:649:HIS:HB2	1:A:653:LYS:O	2.07	0.55
1:A:224:GLN:O	1:A:225:HIS:HB2	2.05	0.55
1:A:212:TYR:N	1:A:217:GLN:HE22	2.06	0.54
1:A:203:LEU:HD13	1:A:245:LEU:HD22	1.91	0.52
1:A:637:ILE:HD13	1:A:647:ILE:HD12	1.92	0.51
1:A:506:ARG:HG2	1:A:507:GLY:N	2.26	0.51
1:A:32:MET:SD	1:A:145:ARG:HD3	2.52	0.50
1:A:54:LEU:HD21	1:A:105:VAL:HG22	1.94	0.49
1:A:307:VAL:HA	1:A:310:MET:HE3	1.94	0.49
1:A:36:MET:HG3	1:A:146:TYR:CD2	2.47	0.49
1:A:476:ILE:HB	1:A:576:ALA:HB3	1.95	0.48
1:A:71:ASP:O	1:A:124:ARG:HG2	2.12	0.48
1:A:497:VAL:HG11	1:A:537:LEU:HD21	1.96	0.47
1:A:149:LYS:HB2	1:A:149:LYS:NZ	2.31	0.46
1:A:478:SER:O	1:A:572:ARG:HA	2.15	0.45
1:A:544:GLY:O	1:A:558:VAL:HG22	2.16	0.45
2:A:2000:MAN:C6	3:A:2001:RAM:H2	2.46	0.45
1:A:536:SER:HB2	1:A:566:TRP:CE2	2.52	0.45
1:A:649:HIS:HD2	9:A:3437:HOH:O	2.00	0.45
1:A:52:LYS:O	1:A:55:ASN:ND2	2.50	0.44
1:A:252:THR:HB	1:A:253:PRO:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:LEU:HA	1:A:228:GLN:O	2.17	0.44
1:A:221:SER:HB3	1:A:343:PHE:CD2	2.52	0.44
1:A:521:LEU:HB2	1:A:592:ILE:HD11	2.00	0.44
1:A:626:THR:HA	1:A:642:PRO:HG3	2.00	0.43
1:A:600:PRO:HG3	1:A:614:HIS:CD2	2.54	0.43
1:A:315:HIS:HE1	9:A:3503:HOH:O	2.01	0.43
1:A:133:THR:HB	1:A:134:PRO:HD3	2.01	0.42
1:A:169:GLU:CD	1:A:169:GLU:H	2.22	0.42
1:A:468:GLU:HB3	1:A:583:LEU:CD2	2.48	0.42
1:A:66:VAL:HA	1:A:67:PRO:HD3	1.88	0.42
1:A:603:LEU:CD1	1:A:630:LEU:HD11	2.49	0.42
1:A:203:LEU:O	1:A:206:PRO:HD2	2.20	0.42
1:A:36:MET:O	1:A:40:LYS:HG2	2.19	0.42
1:A:50:ALA:O	1:A:54:LEU:HB2	2.20	0.42
1:A:306:LEU:HA	1:A:306:LEU:HD12	1.94	0.41
1:A:360:VAL:HG22	1:A:388:THR:HG22	2.02	0.41
1:A:415:ARG:HD3	1:A:480:ALA:CB	2.50	0.41
1:A:44:ARG:O	1:A:45:ASN:HB2	2.21	0.41
1:A:210:VAL:HB	1:A:213:GLU:HG2	2.01	0.41
1:A:302:LYS:HA	1:A:305:LEU:HB2	2.02	0.41
1:A:415:ARG:HD3	1:A:480:ALA:HB3	2.02	0.41
1:A:212:TYR:H	1:A:217:GLN:NE2	2.13	0.41
1:A:529:PHE:CE2	1:A:535:LEU:HD21	2.55	0.41
1:A:95:LYS:HA	1:A:100:TYR:CG	2.56	0.40
1:A:413:THR:HA	1:A:485:THR:O	2.20	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	673/678 (99%)	633 (94%)	38 (6%)	2 (0%)	43	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	HIS
1	A	212	TYR

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	563/578 (97%)	550 (98%)	13 (2%)	53 47

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	137	LEU
1	A	149	LYS
1	A	169	GLU
1	A	201	LYS
1	A	306	LEU
1	A	313	LEU
1	A	401	MET
1	A	404	TRP
1	A	468	GLU
1	A	509	ILE
1	A	543	LYS
1	A	675	LEU

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

Mol	Chain	Res	Type
1	A	55	ASN
1	A	79	ASN
1	A	108	GLN
1	A	217	GLN
1	A	315	HIS

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Mol	Chain	Res	Type
1	A	551	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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$
2	MAN	A	2000	3,4	11,11,12	0.42	0	15,15,17	0.62	0
3	RAM	A	2001	2	9,10,11	1.21	1 (11%)	13,14,16	0.79	0
4	GCU	A	2002	2,5	9,12,13	0.79	0	12,17,19	0.61	0
5	XYP	A	2003	4,6	9,9,10	3.02	3 (33%)	10,12,14	3.07	4 (40%)
6	MFU	A	2004	5	9,10,12	1.29	1 (11%)	13,14,17	0.75	0
8	GOL	A	2010	-	5,5,5	0.32	0	5,5,5	0.29	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	MAN	A	2000	3,4	-	2/2/19/22	0/1/1/1
3	RAM	A	2001	2	-	-	0/1/1/1
4	GCU	A	2002	2,5	-	0/0/21/24	0/1/1/1
5	XYP	A	2003	4,6	-	-	0/1/1/1
6	MFU	A	2004	5	-	-	0/1/1/1
8	GOL	A	2010	-	-	3/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2003	XYP	O5B-C5B	-6.04	1.31	1.42
5	A	2003	XYP	C2B-C3B	5.46	1.60	1.52
6	A	2004	MFU	O5-C1	3.17	1.48	1.43
5	A	2003	XYP	C1B-C2B	2.55	1.58	1.52
3	A	2001	RAM	C4-C5	2.40	1.57	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2003	XYP	C5B-O5B-C1B	8.24	124.20	111.52
5	A	2003	XYP	O2B-C2B-C1B	2.62	114.49	109.17
5	A	2003	XYP	O3B-C3B-C2B	-2.47	105.44	110.02
5	A	2003	XYP	O4B-C4B-C5B	2.04	113.31	109.17

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	2010	GOL	C1-C2-C3-O3
2	A	2000	MAN	O5-C5-C6-O6
2	A	2000	MAN	C4-C5-C6-O6
8	A	2010	GOL	O2-C2-C3-O3
8	A	2010	GOL	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2000	MAN	2	0
3	A	2001	RAM	2	0
4	A	2002	GCU	1	0

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	675/678 (99%)	0.20	43 (6%) 19 22	15, 28, 45, 61	113 (16%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	592	ILE	5.8
1	A	155	LEU	5.2
1	A	504	THR	5.2
1	A	57	LEU	4.6
1	A	151	LEU	4.6
1	A	156	VAL	4.3
1	A	56	THR	4.0
1	A	387	ALA	3.4
1	A	154	ALA	3.3
1	A	597	GLY	3.2
1	A	593	LYS	3.1
1	A	58	GLN	2.8
1	A	50	ALA	2.7
1	A	360	VAL	2.7
1	A	193	GLU	2.7
1	A	144	MET	2.6
1	A	150	PRO	2.5
1	A	49	VAL	2.5
1	A	386	GLY	2.5
1	A	189	LEU	2.4
1	A	584	PRO	2.4
1	A	616	GLN	2.4
1	A	26	GLY	2.4
1	A	412	ILE	2.3
1	A	411	GLY	2.3
1	A	388	THR	2.3
1	A	595	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	651	ASN	2.3
1	A	54	LEU	2.3
1	A	149	LYS	2.2
1	A	652	GLY	2.2
1	A	503	LYS	2.2
1	A	500	THR	2.2
1	A	106	PHE	2.2
1	A	501	ALA	2.2
1	A	554	SER	2.1
1	A	104	LYS	2.1
1	A	191	SER	2.1
1	A	153	GLU	2.0
1	A	410	PRO	2.0
1	A	60	ASP	2.0
1	A	418	LEU	2.0
1	A	650	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 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(\AA^2)	Q<0.9
5	XYP	A	2003	9/10	0.77	0.24	39,40,42,42	9
2	MAN	A	2000	11/12	0.87	0.21	41,45,51,52	0
4	GCU	A	2002	12/13	0.95	0.09	28,40,45,46	0
6	MFU	A	2004	11/12	-	-	43,44,44,44	11
3	RAM	A	2001	10/11	0.36	0.31	48,49,51,51	10
8	GOL	A	2010	6/6	0.91	0.19	28,35,38,39	0
7	CA	A	3000	1/1	0.98	0.04	30,30,30,30	0

6.5 Other polymers ⓘ

There are no such residues in this entry.