



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:40 AM UTC

PDB ID : 6QQM / pdb_00006qqm
Title : Crystal structure of the alpha carbonic anhydrase from Schistosoma mansoni
Authors : Ferraroni, M.; Angeli, A.; Supuran, C.T.
Deposited on : 2019-02-18
Resolution : 1.75 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

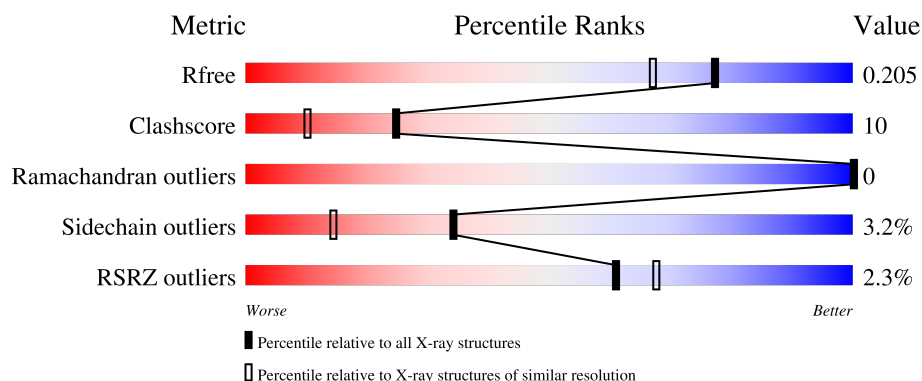
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	300	
1	B	300	

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
4	NAG	A	405	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4955 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 Putative carbonic anhydrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	5	0
			2260	1442	384	426	8			
1	B	277	Total	C	N	O	S	0	3	0
			2236	1426	380	423	7			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP G4VLX3
A	2	THR	-	expression tag	UNP G4VLX3
A	3	TYR	-	expression tag	UNP G4VLX3
A	4	GLN	-	expression tag	UNP G4VLX3
A	5	TRP	-	expression tag	UNP G4VLX3
A	6	LEU	-	expression tag	UNP G4VLX3
A	7	ILE	-	expression tag	UNP G4VLX3
A	8	GLY	-	expression tag	UNP G4VLX3
A	9	ILE	-	expression tag	UNP G4VLX3
A	10	GLN	-	expression tag	UNP G4VLX3
A	11	ILE	-	expression tag	UNP G4VLX3
A	12	SER	-	expression tag	UNP G4VLX3
A	13	LEU	-	expression tag	UNP G4VLX3
A	14	LEU	-	expression tag	UNP G4VLX3
A	15	PHE	-	expression tag	UNP G4VLX3
A	16	VAL	-	expression tag	UNP G4VLX3
A	17	ASN	-	expression tag	UNP G4VLX3
A	18	CYS	-	expression tag	UNP G4VLX3
A	19	ILE	-	expression tag	UNP G4VLX3
A	20	CYS	-	expression tag	UNP G4VLX3
A	21	ASN	-	expression tag	UNP G4VLX3
A	22	GLY	-	expression tag	UNP G4VLX3
A	23	SER	-	expression tag	UNP G4VLX3
A	24	GLU	-	expression tag	UNP G4VLX3
A	25	TRP	-	expression tag	UNP G4VLX3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	26	SER	-	expression tag	UNP G4VLX3
A	27	TYR	-	expression tag	UNP G4VLX3
A	28	THR	-	expression tag	UNP G4VLX3
A	29	ASN	-	expression tag	UNP G4VLX3
A	30	ILE	-	expression tag	UNP G4VLX3
A	31	LEU	-	expression tag	UNP G4VLX3
A	32	THR	-	expression tag	UNP G4VLX3
A	33	GLY	-	expression tag	UNP G4VLX3
A	34	PRO	-	expression tag	UNP G4VLX3
A	35	GLU	-	expression tag	UNP G4VLX3
A	36	THR	-	expression tag	UNP G4VLX3
A	37	TRP	-	expression tag	UNP G4VLX3
A	38	HIS	-	expression tag	UNP G4VLX3
A	39	GLU	-	expression tag	UNP G4VLX3
A	40	HIS	-	expression tag	UNP G4VLX3
A	41	TYR	-	expression tag	UNP G4VLX3
A	42	LYS	-	expression tag	UNP G4VLX3
A	43	ASN	-	expression tag	UNP G4VLX3
A	299	ARG	SER	conflict	UNP G4VLX3
A	300	GLY	SER	conflict	UNP G4VLX3
B	1	MET	-	initiating methionine	UNP G4VLX3
B	2	THR	-	expression tag	UNP G4VLX3
B	3	TYR	-	expression tag	UNP G4VLX3
B	4	GLN	-	expression tag	UNP G4VLX3
B	5	TRP	-	expression tag	UNP G4VLX3
B	6	LEU	-	expression tag	UNP G4VLX3
B	7	ILE	-	expression tag	UNP G4VLX3
B	8	GLY	-	expression tag	UNP G4VLX3
B	9	ILE	-	expression tag	UNP G4VLX3
B	10	GLN	-	expression tag	UNP G4VLX3
B	11	ILE	-	expression tag	UNP G4VLX3
B	12	SER	-	expression tag	UNP G4VLX3
B	13	LEU	-	expression tag	UNP G4VLX3
B	14	LEU	-	expression tag	UNP G4VLX3
B	15	PHE	-	expression tag	UNP G4VLX3
B	16	VAL	-	expression tag	UNP G4VLX3
B	17	ASN	-	expression tag	UNP G4VLX3
B	18	CYS	-	expression tag	UNP G4VLX3
B	19	ILE	-	expression tag	UNP G4VLX3
B	20	CYS	-	expression tag	UNP G4VLX3
B	21	ASN	-	expression tag	UNP G4VLX3
B	22	GLY	-	expression tag	UNP G4VLX3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	23	SER	-	expression tag	UNP G4VLX3
B	24	GLU	-	expression tag	UNP G4VLX3
B	25	TRP	-	expression tag	UNP G4VLX3
B	26	SER	-	expression tag	UNP G4VLX3
B	27	TYR	-	expression tag	UNP G4VLX3
B	28	THR	-	expression tag	UNP G4VLX3
B	29	ASN	-	expression tag	UNP G4VLX3
B	30	ILE	-	expression tag	UNP G4VLX3
B	31	LEU	-	expression tag	UNP G4VLX3
B	32	THR	-	expression tag	UNP G4VLX3
B	33	GLY	-	expression tag	UNP G4VLX3
B	34	PRO	-	expression tag	UNP G4VLX3
B	35	GLU	-	expression tag	UNP G4VLX3
B	36	THR	-	expression tag	UNP G4VLX3
B	37	TRP	-	expression tag	UNP G4VLX3
B	38	HIS	-	expression tag	UNP G4VLX3
B	39	GLU	-	expression tag	UNP G4VLX3
B	40	HIS	-	expression tag	UNP G4VLX3
B	41	TYR	-	expression tag	UNP G4VLX3
B	42	LYS	-	expression tag	UNP G4VLX3
B	43	ASN	-	expression tag	UNP G4VLX3
B	299	ARG	SER	conflict	UNP G4VLX3
B	300	GLY	SER	conflict	UNP G4VLX3

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

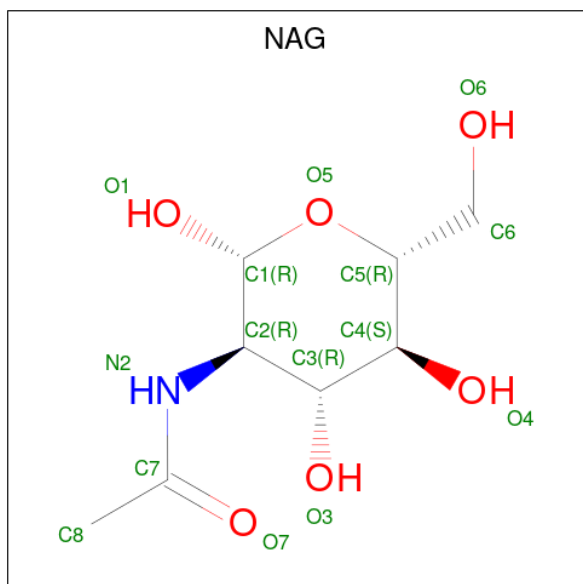
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0

- 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	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

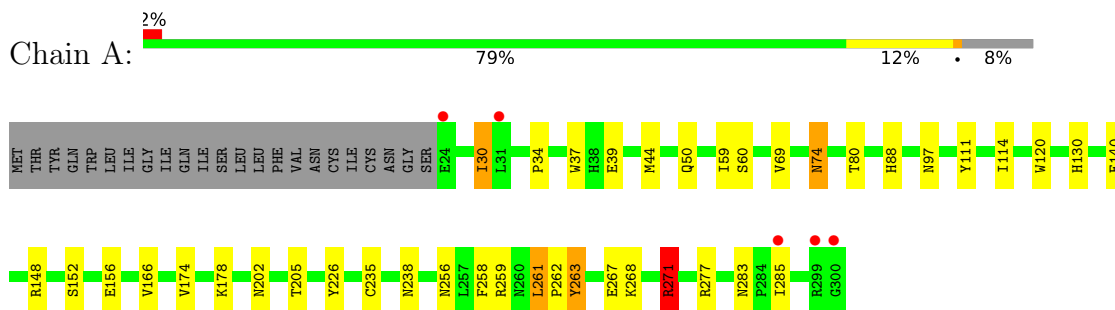
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	206	Total	O	0	0
			206	206		
5	B	183	Total	O	0	0
			183	183		

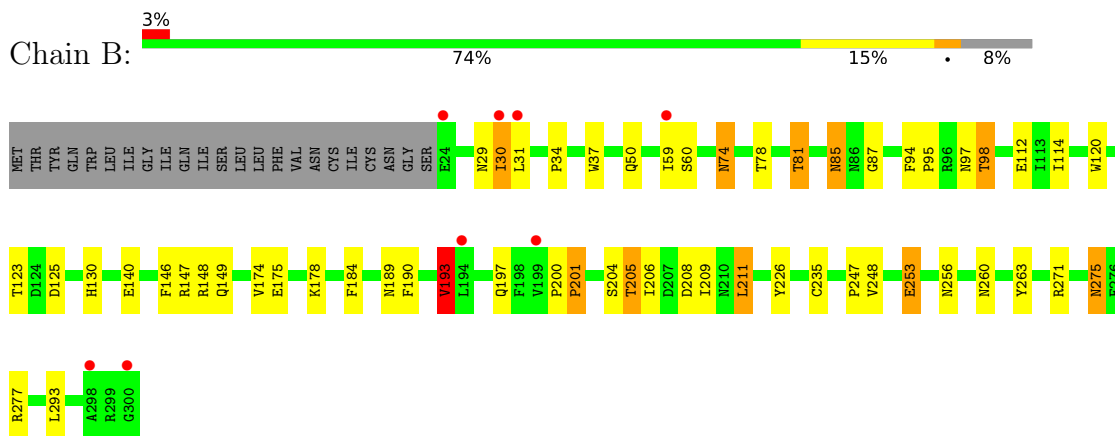
3 Residue-property plots [i](#)

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: Putative carbonic anhydrase



- Molecule 1: Putative carbonic anhydrase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	103.04Å 103.04Å 132.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.60 – 1.75 39.60 – 1.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.60-1.75) 100.0 (39.60-1.75)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 1.75Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.170 , 0.204 0.172 , 0.205	Depositor DCC
R_{free} test set	4301 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 31.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4955	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: GOL, NAG, ZN

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	1.36	10/2335 (0.4%)	1.22	3/3176 (0.1%)
1	B	1.33	6/2305 (0.3%)	1.27	13/3140 (0.4%)
All	All	1.35	16/4640 (0.3%)	1.25	16/6316 (0.3%)

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	B	0	1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	29	ASN	C-N	-9.11	1.24	1.34
1	B	211	LEU	C-N	-7.40	1.24	1.33
1	A	238	ASN	C-O	6.32	1.30	1.24
1	A	283	ASN	C-O	5.94	1.30	1.24
1	A	261	LEU	C-O	-5.83	1.16	1.24
1	B	293	LEU	CA-C	5.58	1.59	1.52
1	A	261	LEU	C-N	5.53	1.40	1.33
1	A	271	ARG	C-O	-5.33	1.17	1.23
1	B	78	THR	C-N	-5.30	1.26	1.33
1	A	262	PRO	N-CD	5.20	1.55	1.47
1	B	248	VAL	N-CA	5.19	1.52	1.46
1	B	201	PRO	N-CD	5.18	1.55	1.47
1	A	30	ILE	C-N	-5.15	1.26	1.34
1	A	69	VAL	CA-C	5.13	1.58	1.52
1	A	74	ASN	C-O	-5.13	1.17	1.24
1	A	166	VAL	N-CA	5.13	1.52	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	200	PRO	C-N-CD	8.57	139.45	120.60
1	B	205[A]	THR	N-CA-C	7.17	120.63	110.23
1	B	205[B]	THR	N-CA-C	7.17	120.63	110.23
1	B	256	ASN	N-CA-C	6.93	119.68	111.71
1	B	114	ILE	CB-CA-C	-6.34	105.42	111.44
1	B	94	PHE	CA-C-N	-6.25	113.84	120.03
1	B	94	PHE	C-N-CA	-6.25	113.84	120.03
1	B	205[A]	THR	CA-C-O	-5.89	114.70	121.47
1	B	205[B]	THR	CA-C-O	-5.89	114.70	121.47
1	B	204	SER	CA-C-N	-5.61	112.74	120.71
1	B	204	SER	C-N-CA	-5.61	112.74	120.71
1	A	261	LEU	CA-C-N	-5.35	114.21	119.99
1	A	261	LEU	C-N-CA	-5.35	114.21	119.99
1	B	193	VAL	N-CA-C	5.30	117.72	111.09
1	A	114	ILE	CB-CA-C	-5.27	106.43	111.44
1	B	211	LEU	CB-CG-CD1	5.18	126.25	110.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	205[B]	THR	Mainchain

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	2260	0	2186	40	0
1	B	2236	0	2145	46	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	12	0	14	3	0
4	A	28	0	26	9	0
4	B	28	0	26	6	0
5	A	206	0	0	12	0
5	B	183	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4955	0	4397	88	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 10.

All (88) 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:74:ASN:ND2	4:A:405:NAG:C1	1.68	1.56
1:A:97:ASN:HB3	4:A:405:NAG:H83	1.35	1.02
1:B:97:ASN:HB3	4:B:403:NAG:H83	1.47	0.96
1:A:152:SER:HB2	1:A:156:GLU:OE2	1.68	0.94
1:A:148:ARG:HH12	4:A:405:NAG:H81	1.37	0.89
1:A:97:ASN:HB3	4:A:405:NAG:C8	2.09	0.81
1:A:59:ILE:C	5:A:504:HOH:O	2.24	0.81
3:A:402:GOL:H32	5:A:622:HOH:O	1.83	0.78
1:B:148:ARG:HH12	4:B:403:NAG:H81	1.47	0.77
1:B:97:ASN:HB3	4:B:403:NAG:C8	2.15	0.76
4:B:402:NAG:O4	5:B:501:HOH:O	2.03	0.75
1:A:50:GLN:HE22	1:A:235:CYS:HB3	1.50	0.75
1:B:59:ILE:CG1	5:B:508:HOH:O	2.35	0.75
1:B:190:PHE:HA	5:B:507:HOH:O	1.88	0.73
1:A:130:HIS:HE1	1:A:226:TYR:OH	1.74	0.70
1:A:74:ASN:ND2	4:A:405:NAG:C2	2.55	0.70
1:A:148:ARG:NH1	4:A:405:NAG:H81	2.05	0.70
1:B:120:TRP:H	1:B:275:ASN:HD21	1.38	0.69
1:B:50:GLN:HE22	1:B:235:CYS:HB3	1.57	0.69
1:B:85:ASN:HD22	1:B:85:ASN:C	2.01	0.69
3:A:402:GOL:C3	5:A:622:HOH:O	2.38	0.68
1:B:130:HIS:HE1	1:B:226:TYR:OH	1.75	0.68
1:B:81:THR:HG21	1:B:208:ASP:OD1	1.94	0.67
1:B:275:ASN:HD22	1:B:275:ASN:H	1.45	0.63
1:B:130:HIS:HD2	1:B:140:GLU:OE2	1.83	0.61
1:A:174:VAL:HG12	1:B:174:VAL:HG12	1.83	0.60
1:B:120:TRP:H	1:B:275:ASN:ND2	1.98	0.60
1:B:50:GLN:NE2	1:B:277:ARG:HH12	1.99	0.60
1:A:111:TYR:OH	5:A:501:HOH:O	2.15	0.58
1:B:85:ASN:ND2	1:B:87:GLY:H	2.00	0.58
1:A:50:GLN:NE2	1:A:277:ARG:HH12	2.02	0.58
1:B:148:ARG:NH1	4:B:403:NAG:H81	2.19	0.58
1:B:123:THR:OG1	1:B:125:ASP:OD1	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:THR:OG1	1:A:205:THR:HG23	2.04	0.57
1:A:130:HIS:HD2	1:A:140:GLU:OE2	1.87	0.57
1:A:60:SER:N	5:A:504:HOH:O	2.37	0.56
1:A:148:ARG:HH12	4:A:405:NAG:C8	2.16	0.56
1:B:81:THR:HG22	5:B:586:HOH:O	2.05	0.55
1:B:147:ARG:HE	1:B:149:GLN:HE21	1.54	0.55
3:A:402:GOL:O3	1:B:247:PRO:O	2.23	0.55
1:B:95:PRO:HG2	1:B:98:THR:HG21	1.89	0.55
1:B:85:ASN:HD22	1:B:87:GLY:H	1.56	0.54
1:B:275:ASN:HD22	1:B:275:ASN:N	2.07	0.53
1:A:263:TYR:CD1	1:A:267:GLU:HG3	2.44	0.53
1:A:59:ILE:HB	5:A:504:HOH:O	2.09	0.53
1:A:74:ASN:ND2	4:A:405:NAG:O5	2.35	0.52
1:A:30:ILE:H	1:A:268:LYS:NZ	2.08	0.52
1:A:271:ARG:CZ	5:A:522:HOH:O	2.58	0.52
1:A:97:ASN:CB	4:A:405:NAG:H83	2.23	0.51
1:B:59:ILE:CG1	5:B:680:HOH:O	2.58	0.51
1:B:260:ASN:HD22	1:B:271:ARG:HH22	1.58	0.51
1:A:271:ARG:HB3	5:A:578:HOH:O	2.10	0.50
1:A:202:ASN:HD22	1:A:202:ASN:N	2.10	0.50
1:A:30:ILE:H	1:A:268:LYS:HZ1	1.59	0.50
1:A:271:ARG:NH2	5:A:510:HOH:O	2.43	0.50
1:A:50:GLN:HE21	1:A:277:ARG:HH22	1.58	0.49
1:B:50:GLN:HE21	1:B:277:ARG:HH22	1.60	0.48
1:B:30:ILE:HD12	1:B:31:LEU:N	2.28	0.48
1:B:275:ASN:H	1:B:275:ASN:ND2	2.11	0.48
1:B:253:GLU:H	1:B:253:GLU:CD	2.22	0.48
1:A:59:ILE:CB	5:A:504:HOH:O	2.62	0.46
5:A:611:HOH:O	1:B:175:GLU:HG2	2.15	0.46
1:B:85:ASN:C	1:B:85:ASN:ND2	2.71	0.46
1:B:147:ARG:HE	1:B:149:GLN:NE2	2.14	0.46
1:A:34:PRO:HA	1:A:37:TRP:CE2	2.52	0.45
1:B:148:ARG:HH12	4:B:403:NAG:C8	2.22	0.45
1:B:209:ILE:HG22	1:B:211:LEU:HD23	1.97	0.45
1:B:34:PRO:HA	1:B:37:TRP:CE2	2.52	0.45
1:A:178:LYS:HE2	5:B:656:HOH:O	2.16	0.44
1:A:256:ASN:HD22	1:A:259:ARG:HD2	1.82	0.44
1:A:120:TRP:CE2	1:A:258:PHE:HB3	2.52	0.43
1:B:81:THR:CG2	5:B:586:HOH:O	2.64	0.43
1:B:60:SER:N	5:B:508:HOH:O	2.52	0.42
1:B:190:PHE:O	1:B:193:VAL:HB	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:LYS:HD3	5:B:656:HOH:O	2.20	0.42
1:B:95:PRO:O	1:B:98:THR:HG23	2.18	0.42
1:A:50:GLN:HE22	1:A:235:CYS:CB	2.26	0.42
1:A:178:LYS:CD	5:B:656:HOH:O	2.67	0.42
1:B:50:GLN:HE21	1:B:277:ARG:HH12	1.68	0.41
1:A:268:LYS:HB2	1:A:268:LYS:HE3	1.92	0.41
1:B:184:PHE:HD2	1:B:189:ASN:HD22	1.67	0.41
1:B:206:ILE:HD12	5:B:507:HOH:O	2.20	0.41
1:A:88:HIS:HB3	5:A:515:HOH:O	2.21	0.41
1:A:261:LEU:HD12	1:A:261:LEU:N	2.36	0.41
1:B:74:ASN:C	1:B:74:ASN:ND2	2.79	0.41
1:B:74:ASN:C	1:B:74:ASN:HD22	2.28	0.40
1:B:112:GLU:HB3	1:B:146:PHE:CE1	2.56	0.40
1:A:44[A]:MET:HB3	1:A:44[A]:MET:HE2	1.66	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	280/300 (93%)	269 (96%)	11 (4%)	0	100	100
1	B	278/300 (93%)	268 (96%)	10 (4%)	0	100	100
All	All	558/600 (93%)	537 (96%)	21 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	254/272 (93%)	250 (98%)	4 (2%)	55	38
1	B	248/272 (91%)	236 (95%)	12 (5%)	23	6
All	All	502/544 (92%)	486 (97%)	16 (3%)	34	14

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLU
1	A	263	TYR
1	A	271	ARG
1	A	285	ILE
1	B	30	ILE
1	B	74	ASN
1	B	81	THR
1	B	85	ASN
1	B	98	THR
1	B	178	LYS
1	B	193	VAL
1	B	197	GLN
1	B	201	PRO
1	B	253	GLU
1	B	263	TYR
1	B	275	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	88	HIS
1	A	130	HIS
1	A	188	ASN
1	A	202	ASN
1	A	256	ASN
1	A	260	ASN
1	B	38	HIS
1	B	43	ASN
1	B	50	GLN
1	B	85	ASN

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Mol	Chain	Res	Type
1	B	122	ASN
1	B	130	HIS
1	B	149	GLN
1	B	260	ASN
1	B	269	GLN
1	B	275	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are 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	$\# Z > 2$
4	NAG	A	405	-	14,14,15	1.02	0	17,19,21	2.41	5 (29%)
3	GOL	A	403	-	5,5,5	1.10	0	5,5,5	1.12	0
3	GOL	A	402	-	5,5,5	1.15	0	5,5,5	1.34	1 (20%)
4	NAG	B	402	-	14,14,15	1.01	2 (14%)	17,19,21	1.05	2 (11%)
4	NAG	A	404	-	14,14,15	0.55	0	17,19,21	2.48	5 (29%)
4	NAG	B	403	-	14,14,15	0.70	0	17,19,21	1.09	1 (5%)

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
4	NAG	A	405	-	-	3/6/23/26	0/1/1/1
3	GOL	A	403	-	-	2/4/4/4	-
3	GOL	A	402	-	-	2/4/4/4	-
4	NAG	B	402	-	-	0/6/23/26	0/1/1/1
4	NAG	A	404	-	-	2/6/23/26	0/1/1/1
4	NAG	B	403	-	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	402	NAG	C2-N2	-2.27	1.42	1.46
4	B	402	NAG	O7-C7	-2.17	1.18	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	405	NAG	C1-O5-C5	-6.76	103.12	112.19
4	A	404	NAG	O5-C1-C2	6.16	120.82	111.29
4	A	404	NAG	C1-O5-C5	5.45	119.49	112.19
4	A	405	NAG	C2-N2-C7	4.32	128.69	122.90
4	B	402	NAG	C1-O5-C5	2.98	116.18	112.19
4	A	405	NAG	O5-C1-C2	-2.61	107.25	111.29
4	A	405	NAG	C3-C4-C5	-2.58	105.55	110.23
4	A	405	NAG	O4-C4-C5	2.53	115.57	109.32
4	A	404	NAG	O6-C6-C5	-2.49	102.86	111.33
4	A	404	NAG	C1-C2-N2	-2.43	106.60	110.43
3	A	402	GOL	O2-C2-C1	2.37	118.97	109.18
4	B	403	NAG	O5-C5-C6	2.36	112.25	107.66
4	A	404	NAG	C2-N2-C7	2.27	125.94	122.90
4	B	402	NAG	C3-C4-C5	-2.04	106.53	110.23

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	A	404	NAG	C8-C7-N2-C2
4	A	404	NAG	O7-C7-N2-C2
4	B	403	NAG	O5-C5-C6-O6
4	B	403	NAG	C4-C5-C6-O6
4	A	405	NAG	C8-C7-N2-C2
4	A	405	NAG	O7-C7-N2-C2
4	B	403	NAG	C8-C7-N2-C2
4	B	403	NAG	O7-C7-N2-C2
3	A	403	GOL	C1-C2-C3-O3
3	A	403	GOL	O2-C2-C3-O3
3	A	402	GOL	O1-C1-C2-O2
4	A	405	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	405	NAG	9	0
3	A	402	GOL	3	0
4	B	402	NAG	1	0
4	B	403	NAG	5	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 [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	277/300 (92%)	-0.17	5 (1%) 67 74	11, 21, 41, 63	5 (1%)
1	B	277/300 (92%)	0.04	8 (2%) 53 60	14, 25, 47, 59	3 (1%)
All	All	554/600 (92%)	-0.06	13 (2%) 61 67	11, 23, 45, 63	8 (1%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	31	LEU	3.6
1	B	300	GLY	3.5
1	B	31	LEU	3.2
1	A	300	GLY	3.2
1	A	285	ILE	2.6
1	B	59	ILE	2.5
1	A	24	GLU	2.3
1	A	299	ARG	2.3
1	B	30	ILE	2.3
1	B	24	GLU	2.2
1	B	199	VAL	2.1
1	B	298	ALA	2.1
1	B	194	LEU	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 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
3	GOL	A	403	6/6	0.73	0.23	44,51,53,56	0
4	NAG	B	403	14/15	0.81	0.13	46,50,55,57	0
4	NAG	A	404	14/15	0.84	0.16	46,56,61,66	0
3	GOL	A	402	6/6	0.85	0.15	19,26,31,35	0
4	NAG	B	402	14/15	0.86	0.12	38,45,54,54	0
4	NAG	A	405	14/15	0.87	0.12	31,44,50,50	0
2	ZN	A	401	1/1	1.00	0.04	19,19,19,19	0
2	ZN	B	401	1/1	1.00	0.05	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.