



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 07:26 PM GMT

PDB ID : 1B5Q
Title : A 30 ANGSTROM U-SHAPED CATALYTIC TUNNEL IN THE CRYSTAL
STRUCTURE OF POLYAMINE OXIDASE
Authors : Binda, C.; Coda, A.; Angelini, R.; Federico, R.; Ascenzi, P.; Mattevi, A.
Deposited on : 1999-01-07
Resolution : 1.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

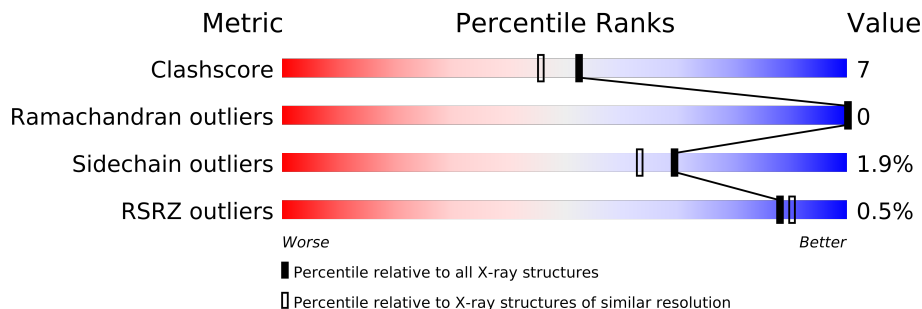
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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))
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	472	
1	B	472	
1	C	472	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	NAG	A	601	-	X
2	NAG	B	601	-	X
2	NAG	B	602	-	X
2	NAG	C	602	-	X
6	MD2	A	590	-	X
6	MD2	B	590	-	X
6	MD2	C	590	-	X

2 Entry composition (i)

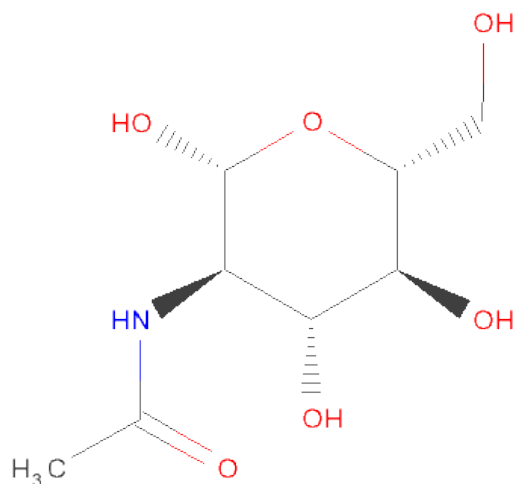
There are 7 unique types of molecules in this entry. The entry contains 12059 atoms, of which 0 are hydrogen and 0 are deuterium.

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 (POLYAMINE OXIDASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	60	0	0
			3684	2353	621	696	14			
1	B	462	Total	C	N	O	S	53	0	0
			3715	2374	627	700	14			
1	C	462	Total	C	N	O	S	44	0	0
			3715	2374	627	700	14			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

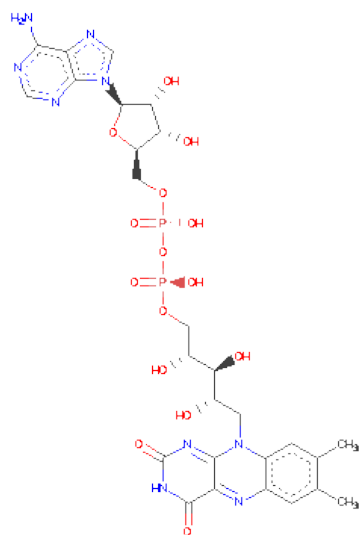
- Molecule 3 is a polymer of unknown type called SUGAR (NAG-NAG).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	2	Total	C	O		0	0
			22	12	10			

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



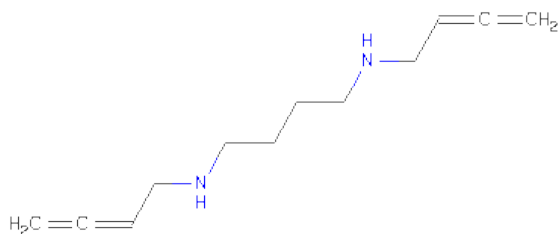
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is N,N'-BIS(2,3-BUTADIENYL)-1,4-BUTANE-DIAMINE (three-letter code: MD2) (formula: C₁₂H₂₀N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	N	0	0
			14	12	2		
6	B	1	Total	C	N	0	0
			14	12	2		
6	C	1	Total	C	N	0	0
			14	12	2		

- Molecule 7 is water.

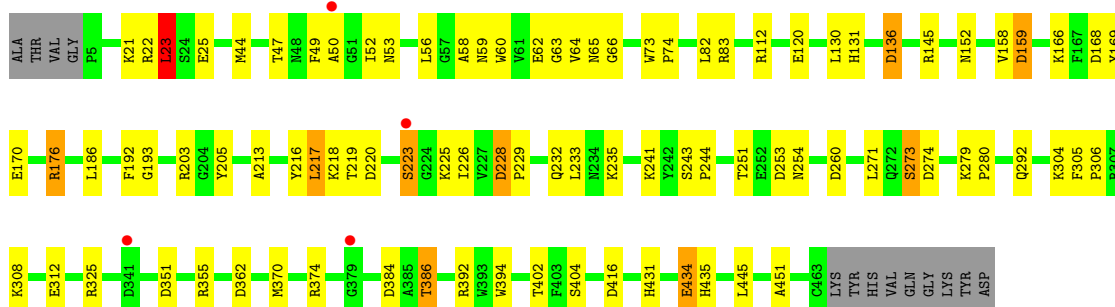
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	195	Total	O	0	0
			195	195		
7	B	207	Total	O	0	0
			207	207		
7	C	226	Total	O	0	0
			226	226		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 (POLYAMINE OXIDASE)

Chain A: 



• Molecule 1: PROTEIN (POLYAMINE OXIDASE)

Chain B: 



• Molecule 1: PROTEIN (POLYAMINE OXIDASE)

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	184.60Å 184.60Å 281.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.0 (50.00-1.90) 96.0 (20.00-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.95 (at 1.90Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.193 , (Not available) 0.188 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 51.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 211139 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12059	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MD2, FCA, NAG, FAD, 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	0.63	0/3775	1.33	35/5116 (0.7%)
1	B	0.64	0/3808	1.31	22/5160 (0.4%)
1	C	0.64	0/3808	1.31	21/5160 (0.4%)
All	All	0.64	0/11391	1.32	78/15436 (0.5%)

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
4	C	1	0

There are no bond length outliers.

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	307	ARG	NE-CZ-NH1	-18.26	111.17	120.30
1	A	355	ARG	NE-CZ-NH2	-15.39	112.61	120.30
1	C	307	ARG	NE-CZ-NH2	14.42	127.51	120.30
1	C	115	LEU	CB-CG-CD1	-12.25	90.18	111.00
1	B	135	ARG	NE-CZ-NH1	-11.46	114.57	120.30
1	B	241	LYS	CD-CE-NZ	10.38	135.57	111.70
1	B	316	ARG	NE-CZ-NH1	10.27	125.43	120.30
1	B	355	ARG	NE-CZ-NH2	-9.78	115.41	120.30
1	B	22	ARG	NE-CZ-NH1	8.89	124.75	120.30
1	C	397	ARG	NE-CZ-NH1	8.29	124.45	120.30
1	C	355	ARG	NE-CZ-NH2	-8.25	116.17	120.30
1	B	424	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	A	355	ARG	NE-CZ-NH1	7.80	124.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ARG	NE-CZ-NH1	-7.79	116.40	120.30
1	A	374	ARG	NE-CZ-NH2	7.77	124.18	120.30
1	C	316	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	A	22	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	A	23	LEU	CB-CG-CD1	7.62	123.95	111.00
1	A	223	SER	CB-CA-C	-7.61	95.64	110.10
1	A	392	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	B	6	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	A	145	ARG	NE-CZ-NH2	7.43	124.02	120.30
1	B	454	LEU	CB-CG-CD1	7.38	123.55	111.00
1	B	325	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	A	416	ASP	CB-CG-OD1	6.99	124.59	118.30
1	A	82	LEU	CB-CG-CD1	-6.83	99.39	111.00
1	C	273	SER	C-N-CA	-6.76	104.80	121.70
1	B	366	LYS	CD-CE-NZ	-6.70	96.28	111.70
1	A	392	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	B	454	LEU	CA-CB-CG	6.50	130.25	115.30
1	C	307	ARG	CD-NE-CZ	-6.45	114.58	123.60
1	B	351	ASP	N-CA-CB	-6.39	99.09	110.60
1	C	86	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	A	159	ASP	CB-CG-OD1	6.33	123.99	118.30
1	A	112	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	B	80	LEU	CB-CG-CD2	-6.21	100.45	111.00
1	C	340	PRO	C-N-CA	-6.21	106.19	121.70
1	B	424	ARG	CG-CD-NE	-6.11	98.97	111.80
1	C	22	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	A	416	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	A	136	ASP	CB-CA-C	-5.94	98.52	110.40
1	A	351	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	386	THR	N-CA-CB	-5.64	99.59	110.30
1	A	374	ARG	NE-CZ-NH1	-5.61	117.49	120.30
1	C	61	VAL	N-CA-C	-5.61	95.86	111.00
1	A	228	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	C	397	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	C	241	LYS	CD-CE-NZ	5.49	124.33	111.70
1	A	325	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	C	150	GLN	CB-CA-C	-5.46	99.49	110.40
1	C	260	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	241	LYS	CD-CE-NZ	5.42	124.16	111.70
1	A	233	LEU	CB-CG-CD1	-5.41	101.80	111.00
1	C	288	ARG	CG-CD-NE	-5.39	100.48	111.80
1	A	83	ARG	NE-CZ-NH1	-5.37	117.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	374	ARG	CG-CD-NE	-5.36	100.54	111.80
1	B	126	LEU	CB-CG-CD2	-5.33	101.93	111.00
1	C	115	LEU	CA-CB-CG	5.33	127.56	115.30
1	B	186	LEU	CB-CG-CD2	-5.30	101.99	111.00
1	B	170	GLU	OE1-CD-OE2	-5.29	116.95	123.30
1	A	260	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	351	ASP	N-CA-CB	-5.18	101.28	110.60
1	A	60	TRP	CB-CA-C	-5.18	100.05	110.40
1	A	273	SER	C-N-CA	-5.15	108.83	121.70
1	A	186	LEU	CB-CG-CD2	-5.14	102.26	111.00
1	A	445	LEU	CB-CG-CD2	-5.13	102.29	111.00
1	B	115	LEU	CB-CG-CD2	-5.11	102.32	111.00
1	A	362	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	86	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	44	MET	N-CA-C	-5.06	97.34	111.00
1	A	251	THR	CA-CB-CG2	-5.05	105.32	112.40
1	B	374	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	C	30	ASP	CB-CG-OD2	5.04	122.83	118.30
1	A	271	LEU	CB-CG-CD1	-5.03	102.45	111.00
1	B	56	LEU	CB-CG-CD1	-5.02	102.46	111.00
1	B	355	ARG	CG-CD-NE	-5.02	101.25	111.80
1	A	176	ARG	CB-CG-CD	-5.01	98.56	111.60
1	C	56	LEU	CB-CG-CD1	-5.01	102.48	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	604	MAN	C1

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3684	0	3585	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3715	0	3614	53	0
1	C	3715	0	3614	35	0
2	A	28	0	26	3	0
2	B	28	0	26	4	0
2	C	14	0	12	1	0
3	C	24	0	21	3	0
4	C	22	0	19	2	0
5	A	53	0	31	2	0
5	B	53	0	31	0	0
5	C	53	0	31	0	0
6	A	14	0	20	4	0
6	B	14	0	20	5	0
6	C	14	0	20	6	0
7	A	195	0	0	7	0
7	B	207	0	0	2	0
7	C	226	0	0	3	0
All	All	12059	0	11070	153	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (153) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:192:PHE:O	7:A:794:HOH:O	1.60	1.19
1:B:69:MET:HE3	1:B:73:TRP:HB3	1.17	1.15
1:B:69:MET:CE	1:B:74:PRO:HD3	1.80	1.10
1:B:69:MET:HE2	1:B:74:PRO:HD3	1.10	1.08
1:B:69:MET:CE	1:B:73:TRP:HB3	1.88	1.02
1:B:69:MET:HE2	1:B:74:PRO:CD	1.94	0.96
1:A:220:ASP:HB3	1:A:223:SER:HB2	1.47	0.94
1:C:131:HIS:CD2	1:C:133:SER:H	1.90	0.88
1:C:91:TYR:OH	1:C:314:LYS:HE2	1.73	0.87
1:A:192:PHE:C	7:A:794:HOH:O	2.05	0.87
2:B:601:NAG:C4	2:B:602:NAG:C1	2.54	0.85
1:B:131:HIS:CD2	1:B:133:SER:H	1.98	0.81
2:A:601:NAG:C4	2:A:602:NAG:C1	2.59	0.80
1:B:131:HIS:HD2	1:B:133:SER:H	1.29	0.76
1:A:273:SER:O	1:A:274:ASP:HB2	1.84	0.76
3:C:601:NAG:C4	2:C:602:NAG:C1	2.64	0.76
1:C:117:ASP:O	1:C:121:GLU:HG3	1.85	0.76
1:A:431:HIS:H	1:A:431:HIS:CD2	2.04	0.75
1:C:404:SER:O	6:C:590:MD2:HC1A	1.86	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:114:GLU:OE1	1:B:114:GLU:HA	1.86	0.74
1:B:69:MET:HE3	1:B:73:TRP:CB	2.10	0.73
1:B:419:ARG:HG2	7:B:777:HOH:O	1.89	0.72
1:B:216:TYR:CD1	1:B:217:LEU:HD13	2.24	0.72
1:B:243:SER:HB2	1:B:244:PRO:HD2	1.73	0.69
1:B:411:ASN:ND2	1:B:414:GLU:H	1.90	0.68
1:A:292:GLN:OE1	7:A:755:HOH:O	2.12	0.68
2:A:601:NAG:HO4	2:A:602:NAG:C1	2.05	0.68
1:A:404:SER:O	6:A:590:MD2:HC1A	1.94	0.68
1:A:223:SER:HB3	1:A:225:LYS:H	1.59	0.67
1:C:148:GLU:OE2	7:C:764:HOH:O	2.13	0.67
1:C:131:HIS:HD2	1:C:133:SER:H	1.40	0.66
1:C:431:HIS:H	1:C:431:HIS:CD2	2.13	0.66
1:B:170:GLU:O	6:B:590:MD2:HC42	1.95	0.66
1:B:69:MET:CE	1:B:74:PRO:CD	2.64	0.65
1:C:170:GLU:O	6:C:590:MD2:HC42	1.96	0.65
1:A:131:HIS:ND1	1:A:136:ASP:OD2	2.30	0.64
1:A:170:GLU:O	6:A:590:MD2:HC42	1.99	0.62
1:A:130:LEU:HD22	1:A:136:ASP:HB2	1.82	0.62
1:B:431:HIS:CD2	1:B:431:HIS:H	2.17	0.62
1:C:131:HIS:HD2	1:C:133:SER:OG	1.82	0.61
3:C:601:NAG:H3	3:C:603:FCA:O2	2.00	0.60
1:A:394:TRP:HE1	1:B:152:ASN:ND2	1.99	0.60
1:A:64:VAL:O	1:A:65:ASN:HB2	2.02	0.58
1:B:243:SER:HB2	1:B:244:PRO:CD	2.34	0.58
1:A:62:GLU:OE2	6:A:590:MD2:HC91	2.02	0.57
1:C:131:HIS:CD2	1:C:133:SER:OG	2.58	0.56
1:A:216:TYR:CD1	1:A:217:LEU:HD13	2.40	0.56
1:B:404:SER:O	6:B:590:MD2:HC1A	2.06	0.56
1:A:169:TYR:CZ	6:A:590:MD2:HC12	2.42	0.55
1:C:405:ASN:OD1	6:C:590:MD2:HC11	2.06	0.55
1:A:273:SER:O	1:A:274:ASP:CB	2.45	0.54
1:A:50:ALA:HB1	1:A:304:LYS:HD2	1.90	0.54
1:C:366:LYS:HD2	1:C:385:ALA:HB3	1.90	0.54
1:A:50:ALA:CB	1:A:304:LYS:HD2	2.38	0.54
1:A:152:ASN:ND2	1:B:394:TRP:HE1	2.06	0.54
1:A:223:SER:CB	1:A:225:LYS:H	2.22	0.53
1:B:244:PRO:O	1:B:424:ARG:NH1	2.40	0.53
1:A:243:SER:HB2	1:A:244:PRO:CD	2.38	0.53
1:A:64:VAL:CA	7:A:794:HOH:O	2.57	0.53
1:A:73:TRP:HB3	1:A:74:PRO:HD3	1.91	0.53
1:B:216:TYR:CE1	1:B:217:LEU:HD13	2.45	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:21:LYS:O	1:A:25:GLU:HG3	2.09	0.52
4:C:604:MAN:H61	4:C:605:MAN:C5	2.39	0.52
1:C:131:HIS:HD2	1:C:133:SER:CB	2.22	0.52
1:A:158:VAL:HG13	1:A:159:ASP:N	2.26	0.51
1:B:411:ASN:HD22	1:B:414:GLU:H	1.55	0.51
1:C:220:ASP:OD2	1:C:222:LYS:N	2.39	0.51
1:B:342:ALA:O	1:B:343:ASN:HB2	2.10	0.51
1:B:273:SER:O	1:B:274:ASP:HB2	2.10	0.51
1:A:23:LEU:HD13	1:A:451:ALA:HB1	1.91	0.51
1:A:394:TRP:HE1	1:B:152:ASN:HD22	1.57	0.51
1:A:431:HIS:CD2	7:A:623:HOH:O	2.63	0.51
4:C:604:MAN:H61	4:C:605:MAN:H5	1.93	0.50
1:C:342:ALA:O	1:C:343:ASN:HB2	2.12	0.50
2:B:601:NAG:H4	2:B:602:NAG:C1	2.39	0.50
1:C:307:ARG:NH1	7:C:767:HOH:O	2.31	0.50
1:C:21:LYS:O	1:C:25:GLU:HG3	2.11	0.50
1:B:148:GLU:O	1:B:149:HIS:HB2	2.11	0.50
1:C:131:HIS:CD2	1:C:133:SER:CB	2.95	0.49
1:C:64:VAL:O	1:C:65:ASN:HB2	2.12	0.49
1:A:434:GLU:HG2	1:A:435:HIS:CD2	2.47	0.49
1:B:131:HIS:CD2	1:B:133:SER:OG	2.66	0.49
1:A:176:ARG:HD2	1:B:177:VAL:HG21	1.95	0.49
1:A:370:MET:HG3	1:A:384:ASP:OD2	2.13	0.49
1:B:216:TYR:CD1	1:B:217:LEU:CD1	2.96	0.48
1:A:216:TYR:CE1	1:A:217:LEU:HD13	2.48	0.48
1:A:66:GLY:N	1:A:192:PHE:O	2.43	0.48
1:B:307:ARG:NH2	1:B:381:ASP:OD2	2.45	0.48
1:C:220:ASP:HB3	1:C:223:SER:OG	2.13	0.48
1:A:235:LYS:NZ	1:A:253:ASP:OD2	2.32	0.48
2:B:601:NAG:HO4	2:B:602:NAG:C1	2.22	0.48
1:B:6:ARG:HA	1:B:30:ASP:O	2.14	0.48
1:A:64:VAL:N	7:A:794:HOH:O	2.46	0.48
1:C:169:TYR:O	6:C:590:MD2:H111	2.13	0.47
1:B:63:GLY:HA2	1:B:193:GLY:O	2.14	0.47
1:B:131:HIS:HD2	1:B:133:SER:N	2.05	0.47
1:B:131:HIS:HD2	1:B:133:SER:OG	1.97	0.47
1:A:49:PHE:O	1:A:52:ILE:HG12	2.14	0.47
1:A:229:PRO:O	1:A:232:GLN:NE2	2.41	0.47
1:C:243:SER:HB2	1:C:244:PRO:CD	2.44	0.47
3:C:601:NAG:C3	3:C:603:FCA:O2	2.63	0.47
1:A:63:GLY:HA2	1:A:193:GLY:O	2.14	0.47
1:C:131:HIS:HD2	1:C:133:SER:N	2.11	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:152:ASN:HD22	1:B:394:TRP:HE1	1.61	0.47
1:B:114:GLU:CA	1:B:114:GLU:OE1	2.58	0.46
1:A:63:GLY:C	7:A:794:HOH:O	2.53	0.46
1:C:403:PHE:CZ	6:C:590:MD2:HC62	2.50	0.46
1:C:238:ARG:NH1	1:C:252:GLU:OE2	2.47	0.46
1:A:218:LYS:H	1:A:228:ASP:HB2	1.80	0.46
1:B:169:TYR:CZ	6:B:590:MD2:HC12	2.51	0.46
1:A:243:SER:CB	1:A:244:PRO:CD	2.94	0.45
1:C:250:LYS:HG2	1:C:256:VAL:HG22	1.97	0.45
1:C:219:THR:HG22	1:C:226:ILE:HA	1.98	0.45
1:A:308:LYS:HD2	1:A:312:GLU:CD	2.37	0.45
1:B:451:ALA:O	1:B:455:ILE:HG13	2.17	0.45
1:A:220:ASP:CB	1:A:223:SER:HB2	2.34	0.44
1:C:173:GLU:OE1	1:C:294:ASP:OD2	2.36	0.44
1:A:47:THR:O	1:A:53:ASN:HA	2.16	0.44
1:B:449:ASP:O	1:B:453:ILE:HG13	2.17	0.44
1:A:73:TRP:N	1:A:74:PRO:CD	2.81	0.44
1:C:439:TYR:CZ	6:C:590:MD2:HC41	2.53	0.43
1:B:419:ARG:HD3	7:B:797:HOH:O	2.18	0.43
1:A:370:MET:HE2	1:A:384:ASP:HA	2.00	0.43
1:C:158:VAL:HG12	7:C:779:HOH:O	2.19	0.43
1:B:69:MET:HE2	1:B:74:PRO:CG	2.48	0.43
1:B:133:SER:O	1:B:411:ASN:HB2	2.18	0.43
1:B:110:GLN:O	1:B:114:GLU:HG2	2.17	0.43
2:A:601:NAG:H4	2:A:602:NAG:C1	2.46	0.43
1:A:219:THR:HG22	1:A:226:ILE:HA	2.01	0.43
1:A:213:ALA:O	1:A:217:LEU:HB2	2.19	0.42
1:C:431:HIS:N	1:C:431:HIS:CD2	2.85	0.42
1:A:47:THR:HG21	1:A:56:LEU:HD21	2.00	0.42
1:B:243:SER:CB	1:B:244:PRO:CD	2.95	0.42
1:A:131:HIS:HD1	1:A:136:ASP:CG	2.23	0.42
1:C:100:ASP:OD1	1:C:375:LYS:HE2	2.19	0.42
1:B:154:PRO:HB3	1:B:159:ASP:HB3	2.00	0.42
1:B:141:LEU:HD22	1:B:176:ARG:HB3	2.01	0.42
1:A:120:GLU:OE1	1:A:166:LYS:NZ	2.45	0.42
1:A:253:ASP:O	1:A:254:ASN:HB2	2.20	0.42
1:C:219:THR:HA	1:C:225:LYS:O	2.18	0.42
1:B:131:HIS:HD2	1:B:133:SER:CB	2.33	0.41
1:A:58:ALA:HA	5:A:579:FAD:C4X	2.50	0.41
2:B:601:NAG:O4	2:B:602:NAG:C2	2.63	0.41
1:A:305:PHE:HB3	1:A:306:PRO:HD2	2.02	0.41
1:B:52:ILE:O	1:B:52:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:279:LYS:HA	1:A:280:PRO:HA	1.90	0.41
1:C:187:ALA:HA	1:C:190:SER:OG	2.20	0.41
1:B:105:ASP:OD1	1:B:108:TYR:N	2.49	0.41
1:B:62:GLU:OE2	6:B:590:MD2:HC91	2.21	0.41
1:A:402:THR:HB	5:A:579:FAD:HM83	2.03	0.40
1:B:439:TYR:CZ	6:B:590:MD2:HC41	2.56	0.40
1:C:141:LEU:HD22	1:C:176:ARG:HB3	2.03	0.40
1:B:216:TYR:CE1	1:B:217:LEU:CD1	3.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	457/472 (97%)	438 (96%)	19 (4%)	0	100	100
1	B	460/472 (98%)	442 (96%)	18 (4%)	0	100	100
1	C	460/472 (98%)	442 (96%)	18 (4%)	0	100	100
All	All	1377/1416 (97%)	1322 (96%)	55 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	394/404 (98%)	387 (98%)	7 (2%)	71	66
1	B	397/404 (98%)	389 (98%)	8 (2%)	68	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	397/404 (98%)	390 (98%)	7 (2%)	71	66
All	All	1188/1212 (98%)	1166 (98%)	22 (2%)	69	63

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	59	ASN
1	A	168	ASP
1	A	205	TYR
1	A	217	LEU
1	A	386	THR
1	A	434	GLU
1	B	59	ASN
1	B	105	ASP
1	B	168	ASP
1	B	205	TYR
1	B	217	LEU
1	B	238	ARG
1	B	411	ASN
1	B	454	LEU
1	C	59	ASN
1	C	105	ASP
1	C	115	LEU
1	C	127	SER
1	C	149	HIS
1	C	168	ASP
1	C	205	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	360	GLN
1	A	431	HIS
1	B	131	HIS
1	B	149	HIS
1	B	152	ASN
1	B	360	GLN
1	B	411	ASN
1	B	431	HIS

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Mol	Chain	Res	Type
1	B	466	HIS
1	C	131	HIS
1	C	360	GLN
1	C	431	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

4 carbohydrates 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	$\# Z > 2$
3	NAG	C	601	1,3,2	12,14,15	1.68	5 (41%)	15,19,21	4.28	9 (60%)
3	FCA	C	603	3	9,10,11	1.33	1 (11%)	10,14,16	2.08	4 (40%)
4	MAN	C	604	2,4	10,11,12	0.57	0	11,15,17	2.17	3 (27%)
4	MAN	C	605	4	10,11,12	0.61	0	11,15,17	1.52	2 (18%)

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	NAG	C	601	1,3,2	-	0/6/23/26	0/1/1/1
3	FCA	C	603	3	-	0/0/17/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	C	604	2,4	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	C	605	4	-	0/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	NAG	C2-N2	2.50	1.49	1.46
3	C	601	NAG	C4-C3	-2.50	1.45	1.52
3	C	603	FCA	C3-C2	-2.49	1.47	1.52
3	C	601	NAG	C6-C5	-2.45	1.43	1.52
3	C	601	NAG	O5-C5	2.15	1.49	1.45
3	C	601	NAG	C3-C2	-2.02	1.48	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	NAG	O5-C5-C6	-8.43	98.14	106.98
3	C	601	NAG	C8-C7-N2	-7.18	102.06	116.11
3	C	601	NAG	O7-C7-C8	6.07	133.89	122.04
4	C	604	MAN	O2-C2-C3	5.57	122.19	110.18
3	C	601	NAG	O6-C6-C5	5.40	129.93	111.36
3	C	601	NAG	C6-C5-C4	5.12	125.36	113.00
3	C	601	NAG	O4-C4-C3	4.44	120.31	110.35
3	C	603	FCA	O5-C5-C6	-4.41	100.95	108.03
3	C	601	NAG	O5-C5-C4	-4.23	105.28	110.65
4	C	604	MAN	O5-C5-C6	3.15	110.29	106.98
3	C	601	NAG	C3-C2-N2	2.96	116.28	111.76
4	C	605	MAN	O2-C2-C3	2.91	116.45	110.18
3	C	603	FCA	C3-C4-C5	-2.75	105.27	109.84
3	C	601	NAG	C3-C4-C5	2.73	115.08	110.20
3	C	603	FCA	O3-C3-C4	-2.59	104.55	110.35
3	C	603	FCA	O3-C3-C2	2.42	114.36	109.94
4	C	605	MAN	C3-C4-C5	-2.34	106.03	110.20
4	C	604	MAN	C3-C4-C5	-2.09	106.48	110.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	604	MAN	C1

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry

11 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	$\# Z > 2$
5	FAD	A	579	-	58,58,58	1.01	2 (3%)	85,89,89	1.77	13 (15%)
6	MD2	A	590	-	13,13,13	0.70	0	12,12,12	1.97	4 (33%)
2	NAG	A	601	1,2	12,14,15	1.62	2 (16%)	15,19,21	3.46	10 (66%)
2	NAG	A	602	2	12,14,15	0.94	1 (8%)	15,19,21	2.42	6 (40%)
5	FAD	B	579	-	58,58,58	0.86	1 (1%)	85,89,89	1.64	10 (11%)
6	MD2	B	590	-	13,13,13	0.75	0	12,12,12	1.47	3 (25%)
2	NAG	B	601	1,2	12,14,15	1.75	4 (33%)	15,19,21	3.24	9 (60%)
2	NAG	B	602	1,2	12,14,15	1.25	1 (8%)	15,19,21	4.08	7 (46%)
5	FAD	C	579	-	58,58,58	1.09	2 (3%)	85,89,89	1.84	9 (10%)
6	MD2	C	590	-	13,13,13	0.72	0	12,12,12	2.26	3 (25%)
2	NAG	C	602	3,4	12,14,15	1.47	3 (25%)	15,19,21	4.29	4 (26%)

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
5	FAD	A	579	-	-	0/34/50/50	0/1/6/6
6	MD2	A	590	-	-	0/9/11/11	0/0/0/0
2	NAG	A	601	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	602	2	-	0/6/23/26	0/1/1/1
5	FAD	B	579	-	-	0/34/50/50	0/1/6/6
6	MD2	B	590	-	-	0/9/11/11	0/0/0/0
2	NAG	B	601	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	602	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FAD	C	579	-	-	0/34/50/50	0/1/6/6
6	MD2	C	590	-	-	0/9/11/11	0/0/0/0
2	NAG	C	602	3,4	-	0/6/23/26	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	579	FAD	C1'-C2'	4.83	1.56	1.51
5	C	579	FAD	C1'-C2'	4.46	1.55	1.51
2	B	601	NAG	O5-C5	4.03	1.52	1.45
2	A	601	NAG	O5-C5	3.89	1.52	1.45
2	B	602	NAG	C2-N2	3.48	1.50	1.46
2	A	601	NAG	O3-C3	2.95	1.50	1.43
5	B	579	FAD	PA-O3P	2.78	1.64	1.59
2	C	602	NAG	O5-C5	2.70	1.50	1.45
2	C	602	NAG	O6-C6	2.68	1.54	1.42
2	B	601	NAG	O3-C3	2.50	1.49	1.43
2	B	601	NAG	C4-C3	-2.19	1.46	1.52
5	A	579	FAD	C4-N3	2.18	1.40	1.37
5	C	579	FAD	C5'-C4'	2.11	1.55	1.51
2	B	601	NAG	C2-N2	2.11	1.48	1.46
2	C	602	NAG	O4-C4	-2.06	1.38	1.43
2	A	602	NAG	C2-N2	2.05	1.48	1.46

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	602	NAG	O5-C5-C6	-13.91	92.39	106.98
2	B	602	NAG	O5-C5-C6	-11.24	95.19	106.98
5	A	579	FAD	C4X-C10-N10	-9.78	115.63	120.51
5	C	579	FAD	C4X-C10-N10	-9.44	115.80	120.51
2	B	602	NAG	O6-C6-C5	8.05	139.05	111.36
2	A	601	NAG	O5-C5-C6	-7.09	99.54	106.98
2	A	601	NAG	O6-C6-C5	6.77	134.65	111.36
5	C	579	FAD	C2-N1-C10	6.75	121.78	114.98
2	C	602	NAG	O5-C5-C4	-6.42	102.50	110.65
5	B	579	FAD	C2-N1-C10	6.36	121.39	114.98
2	B	601	NAG	O5-C5-C4	-6.23	102.75	110.65
2	B	601	NAG	C2-N2-C7	-5.76	113.42	123.09
5	A	579	FAD	C1'-N10-C9A	5.67	124.39	118.87
2	A	602	NAG	C2-N2-C7	-5.38	114.05	123.09
6	C	590	MD2	C4-C3-C2	5.31	135.90	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	579	FAD	O4B-C1B-N9A	-5.24	103.57	108.44
2	C	602	NAG	O4-C4-C3	4.91	121.35	110.35
2	B	601	NAG	O5-C5-C6	-4.86	101.88	106.98
2	B	601	NAG	O6-C6-C5	4.54	126.98	111.36
5	C	579	FAD	O4B-C1B-N9A	-4.44	104.31	108.44
5	C	579	FAD	O4B-C1B-C2B	-4.41	100.02	106.77
6	C	590	MD2	C11-C12-C13	-4.30	115.85	124.81
2	A	602	NAG	O5-C5-C6	4.29	111.48	106.98
5	B	579	FAD	C4A-C5A-N7A	4.11	113.05	109.52
5	C	579	FAD	C8A-N9A-C4A	-4.09	103.78	106.90
5	A	579	FAD	C2-N1-C10	4.04	119.05	114.98
5	C	579	FAD	N3A-C2A-N1A	3.94	132.00	128.71
5	B	579	FAD	O4B-C1B-C2B	-3.77	100.99	106.77
2	A	601	NAG	C8-C7-N2	-3.75	108.78	116.11
5	A	579	FAD	C9A-C5X-N5	-3.70	116.70	122.37
2	B	602	NAG	C6-C5-C4	3.67	121.87	113.00
5	B	579	FAD	C2'-C1'-N10	3.64	117.29	112.45
2	A	601	NAG	C6-C5-C4	3.64	121.80	113.00
2	B	602	NAG	C2-N2-C7	-3.54	117.14	123.09
5	B	579	FAD	C1'-N10-C9A	3.48	122.25	118.87
6	A	590	MD2	C8-C9-N10	-3.40	103.06	112.09
2	A	601	NAG	O7-C7-C8	3.36	128.60	122.04
2	B	602	NAG	O5-C5-C4	-3.26	106.52	110.65
2	A	602	NAG	C3-C2-N2	3.26	116.72	111.76
6	B	590	MD2	C11-C12-C13	-3.25	118.04	124.81
5	B	579	FAD	C4X-C10-N1	-3.23	119.50	122.73
6	A	590	MD2	C11-C12-C13	-3.23	118.08	124.81
2	A	601	NAG	C2-N2-C7	-3.18	117.75	123.09
2	B	601	NAG	O4-C4-C5	-3.18	100.92	109.28
6	A	590	MD2	C4-C3-C2	-3.11	118.32	124.81
5	B	579	FAD	C9A-N10-C10	-3.11	118.72	121.77
6	A	590	MD2	C11-N10-C9	-3.10	102.21	113.47
2	A	601	NAG	O4-C4-C5	-2.95	101.50	109.28
5	A	579	FAD	C5'-C4'-C3'	-2.95	106.48	112.06
2	B	602	NAG	C3-C2-N2	2.81	116.04	111.76
2	B	602	NAG	O4-C4-C3	2.81	116.66	110.35
2	B	601	NAG	O3-C3-C4	2.70	116.40	110.35
5	A	579	FAD	C4A-C5A-N7A	2.68	111.82	109.52
5	C	579	FAD	O3'-C3'-C2'	-2.61	102.14	108.74
2	B	601	NAG	O4-C4-C3	-2.61	104.51	110.35
5	B	579	FAD	C4-N3-C2	-2.60	120.05	125.39
2	A	601	NAG	O3-C3-C4	2.59	116.15	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	602	NAG	O3-C3-C4	2.47	115.88	110.35
2	A	601	NAG	C3-C4-C5	2.42	114.53	110.20
5	A	579	FAD	C9A-N10-C10	-2.42	119.39	121.77
6	C	590	MD2	C4-N5-C6	2.40	122.18	113.47
2	C	602	NAG	O3-C3-C4	2.40	115.73	110.35
5	A	579	FAD	O2'-C2'-C3'	-2.37	103.14	109.05
5	C	579	FAD	C8A-N9A-C1B	2.36	131.03	126.38
2	A	601	NAG	O5-C5-C4	-2.35	107.67	110.65
6	B	590	MD2	C7-C6-N5	2.30	118.21	112.09
2	A	602	NAG	C6-C5-C4	2.30	118.55	113.00
2	B	601	NAG	O7-C7-C8	2.24	126.42	122.04
5	A	579	FAD	C1'-N10-C10	-2.23	116.00	119.17
2	A	602	NAG	O4-C4-C5	2.22	115.13	109.28
5	A	579	FAD	C2B-C3B-C4B	2.22	107.07	102.65
5	A	579	FAD	C6-C5X-C9A	2.21	122.08	119.02
5	B	579	FAD	C6-C7-C8	-2.16	116.42	119.88
5	A	579	FAD	C5X-C9A-N10	2.12	118.89	116.80
5	C	579	FAD	C4'-C3'-C2'	2.09	117.97	113.25
2	B	601	NAG	C3-C4-C5	2.07	113.90	110.20
5	A	579	FAD	C4X-N5-C5X	2.04	118.99	116.69
6	B	590	MD2	C4-C3-C2	-2.00	120.63	124.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	459/472 (97%)	-0.50	4 (0%)	81 83	6, 15, 38, 69	20 (4%)
1	B	462/472 (97%)	-0.59	1 (0%)	93 94	4, 13, 36, 70	18 (3%)
1	C	462/472 (97%)	-0.59	2 (0%)	90 91	5, 12, 36, 57	15 (3%)
All	All	1383/1416 (97%)	-0.56	7 (0%)	88 90	4, 13, 37, 70	53 (3%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	379	GLY	2.7
1	A	50	ALA	2.6
1	A	223	SER	2.5
1	B	466	HIS	2.3
1	A	341	ASP	2.2
1	C	220	ASP	2.2
1	C	222	LYS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	C	601	14/15	0.14	5.46	1,12,24,57	0
3	FCA	C	603	10/11	0.20	3.92	9,34,42,75	0
4	MAN	C	605	11/12	0.29	-	30,40,63,96	0
4	MAN	C	604	11/12	0.23	-	24,36,53,55	0

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MD2	C	590	14/14	0.14	6.59	19,30,38,46	0
6	MD2	B	590	14/14	0.15	6.16	13,33,55,55	0
2	NAG	C	602	14/15	0.21	5.16	3,12,39,74	0
6	MD2	A	590	14/14	0.13	5.04	19,32,39,41	0
2	NAG	B	602	14/15	0.29	4.84	14,46,98,100	0
2	NAG	A	601	14/15	0.15	4.17	17,35,71,100	0
2	NAG	B	601	14/15	0.14	2.76	9,24,38,100	0
5	FAD	B	579	53/53	0.06	-0.30	1,6,9,10	0
5	FAD	A	579	53/53	0.06	-0.68	3,9,13,16	0
5	FAD	C	579	53/53	0.06	-0.75	3,7,12,12	0
2	NAG	A	602	14/15	0.32	-	26,53,100,100	0

6.5 Other polymers

There are no such residues in this entry.