



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:31 am 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 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

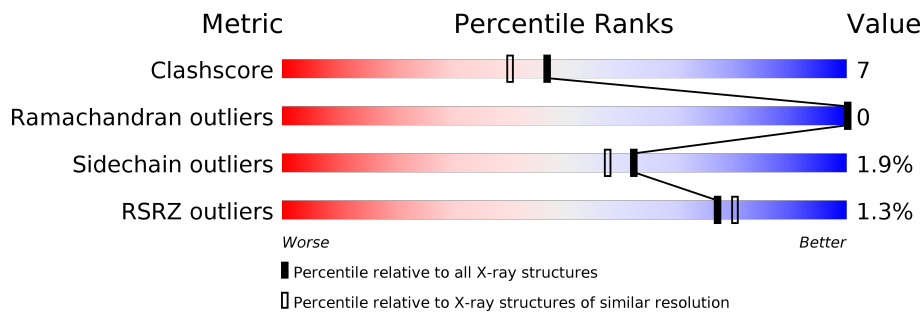
1 Overall quality at a glance

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))
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (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	472	<div> <div></div> <div>78%</div> <div>17%</div> <div>..</div> </div>
1	B	472	<div> <div></div> <div>84%</div> <div>13%</div> <div>..</div> </div>
1	C	472	<div> <div></div> <div>84%</div> <div>14%</div> <div>.</div> </div>

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	MAN	C	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	MD2	A	590	-	-	-	X
6	MD2	B	590	-	-	-	X
6	MD2	C	590	-	-	-	X

2 Entry composition [i](#)

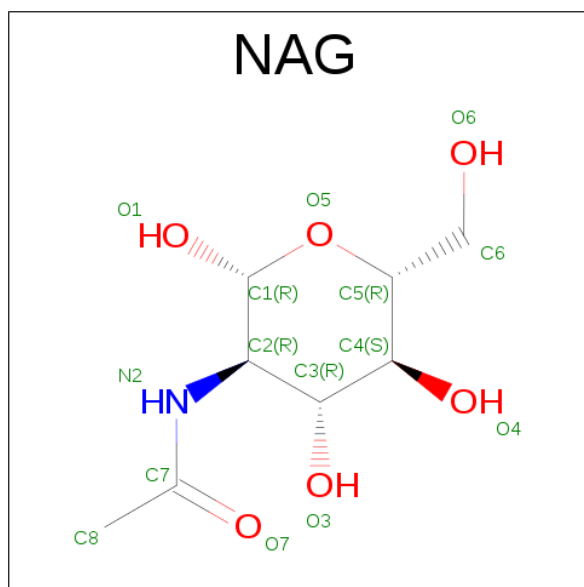
There are 7 unique types of molecules in this entry. The entry contains 12059 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (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		

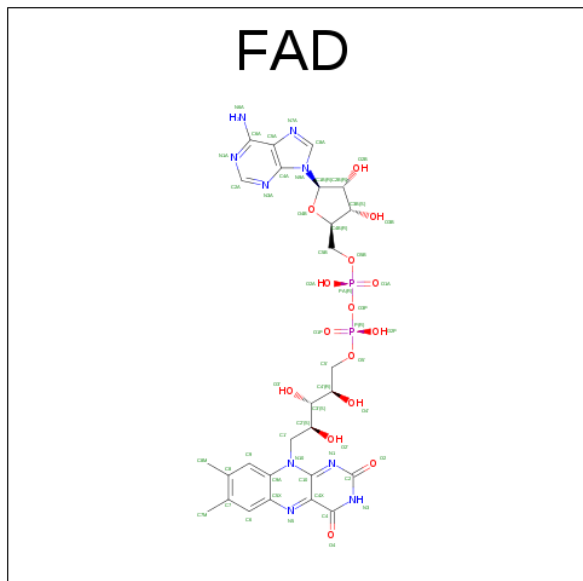
- Molecule 3 is a polymer of unknown type called SUGAR (NAG-NAG).

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: $C_{27}H_{33}N_9O_{15}P_2$).



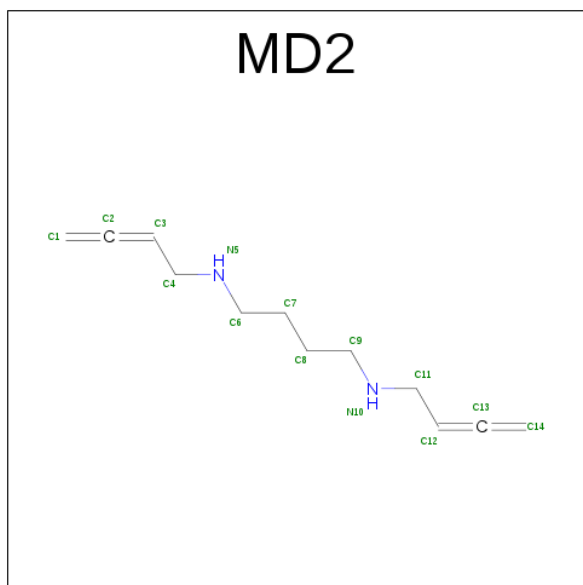
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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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		

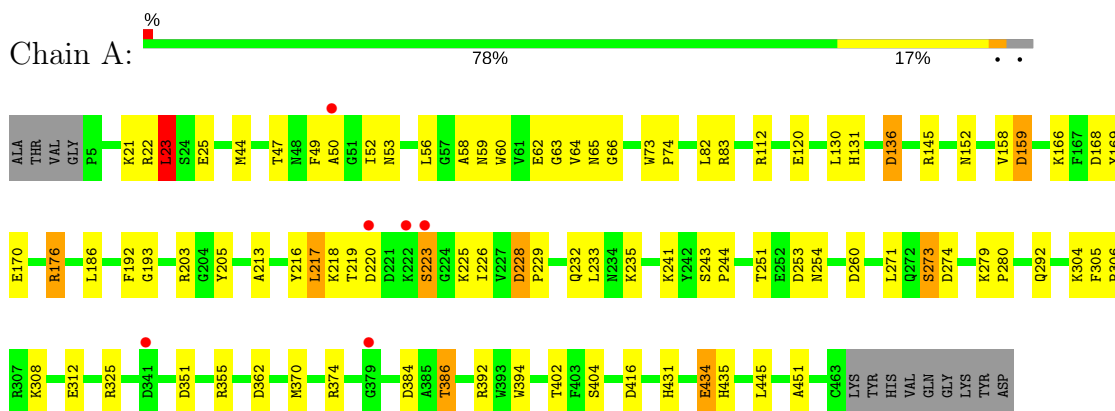
- Molecule 7 is water.

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		

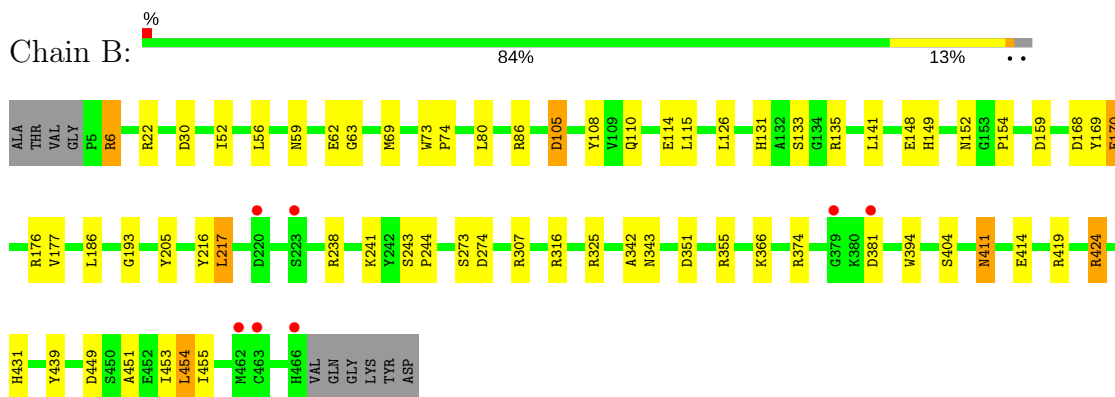
3 Residue-property plots [i](#)

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.

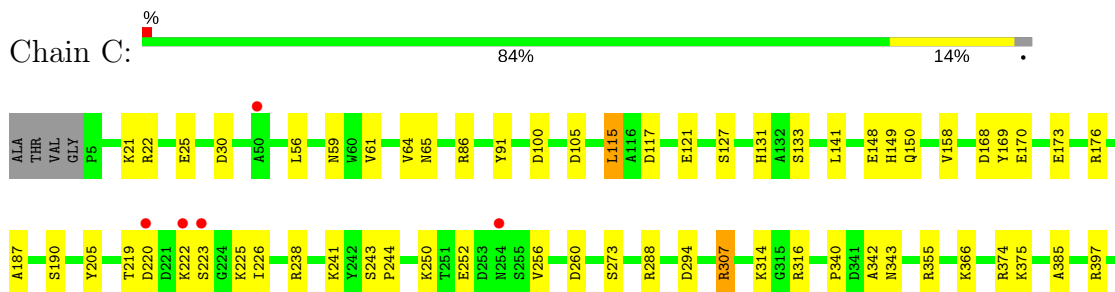
• Molecule 1: PROTEIN (POLYAMINE OXIDASE)



• Molecule 1: PROTEIN (POLYAMINE OXIDASE)



• Molecule 1: PROTEIN (POLYAMINE OXIDASE)



F403	S404	N405	H431	Y439	H466	VAL	GLN	GLY	LYS	TYR	ASP
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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)	0.39 , 71.5	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	0.95	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.

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: 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 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	3684	0	3585	58	0
1	B	3715	0	3614	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 7.

All (153) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:SER:O	6:C:590:MD2:HC1A	1.86	0.74
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:TRP:HB3	1:A:74:PRO:HD3	1.91	0.53
1:A:21:LYS:O	1:A:25:GLU:HG3	2.09	0.52
1:B:216:TYR:CE1	1:B:217:LEU:HD13	2.45	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:273:SER:O	1:B:274:ASP:HB2	2.10	0.51
1:B:342:ALA:O	1:B:343:ASN:HB2	2.10	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: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
1:C:342:ALA:O	1:C:343:ASN:HB2	2.12	0.50
4:C:604:MAN:H61	4:C:605:MAN:H5	1.93	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:370:MET:HG3	1:A:384:ASP:OD2	2.13	0.49
1:A:176:ARG:HD2	1:B:177:VAL:HG21	1.95	0.49
1:A:216:TYR:CE1	1:A:217:LEU:HD13	2.48	0.48
1:B:216:TYR:CD1	1:B:217:LEU:CD1	2.96	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:A:235:LYS:NZ	1:A:253:ASP:OD2	2.32	0.48
1:C:220:ASP:HB3	1:C:223:SER:OG	2.13	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:B:63:GLY:HA2	1:B:193:GLY:O	2.14	0.47
1:C:169:TYR:O	6:C:590:MD2:H111	2.13	0.47
1:A:49:PHE:O	1:A:52:ILE:HG12	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:152:ASN:HD22	1:B:394:TRP:HE1	1.61	0.47
1:C:131:HIS:HD2	1:C:133:SER:N	2.11	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:A:218:LYS:H	1:A:228:ASP:HB2	1.80	0.46
1:C:238:ARG:NH1	1:C:252:GLU:OE2	2.47	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:A:47:THR:O	1:A:53:ASN:HA	2.16	0.44
1:C:173:GLU:OE1	1:C:294:ASP:OD2	2.36	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:110:GLN:O	1:B:114:GLU:HG2	2.17	0.43
1:B:133:SER:O	1:B:411:ASN:HB2	2.18	0.43
1:A:219:THR:HG22	1:A:226:ILE:HA	2.01	0.43
2:A:601:NAG:H4	2:A:602:NAG:C1	2.46	0.43
1:A:213:ALA:O	1:A:217:LEU:HB2	2.19	0.42
1:A:47:THR:HG21	1:A:56:LEU:HD21	2.00	0.42
1:C:431:HIS:N	1:C:431:HIS:CD2	2.85	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:B:154:PRO:HB3	1:B:159:ASP:HB3	2.00	0.42
1:C:100:ASP:OD1	1:C:375:LYS:HE2	2.19	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:A:58:ALA:HA	5:A:579:FAD:C4X	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:HIS:HD2	1:B:133:SER:CB	2.33	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
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%)	64	60
1	B	397/404 (98%)	389 (98%)	8 (2%)	60	55
1	C	397/404 (98%)	390 (98%)	7 (2%)	64	60
All	All	1188/1212 (98%)	1166 (98%)	22 (2%)	62	57

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

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Mol	Chain	Res	Type
1	B	149	HIS
1	B	152	ASN
1	B	360	GLN
1	B	411	ASN
1	B	431	HIS
1	B	466	HIS
1	C	131	HIS
1	C	360	GLN
1	C	431	HIS

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 ⓘ

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	14,14,15	1.78	4 (28%)	15,19,21	4.29	10 (66%)
3	FCA	C	603	3	9,10,11	1.76	1 (11%)	13,14,16	2.13	6 (46%)
4	MAN	C	604	2,4	11,11,12	0.81	0	13,15,17	2.27	4 (30%)
4	MAN	C	605	4	11,11,12	0.75	0	13,15,17	1.82	4 (30%)

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
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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	603	FCA	C2-C3	-3.85	1.47	1.52
3	C	601	NAG	C1-C2	-3.13	1.48	1.52
3	C	601	NAG	C4-C3	-2.60	1.45	1.52
3	C	601	NAG	C6-C5	-2.51	1.43	1.51
3	C	601	NAG	O5-C5	2.83	1.49	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	NAG	C8-C7-N2	-7.78	102.06	116.11
3	C	601	NAG	O5-C1-C2	-3.62	106.44	111.47
4	C	605	MAN	C1-C2-C3	-3.22	105.58	109.65
3	C	603	FCA	O5-C1-C2	-2.89	106.26	110.79
3	C	601	NAG	C1-C2-N2	-2.82	105.68	110.49
3	C	603	FCA	C3-C4-C5	-2.81	105.27	109.68
4	C	604	MAN	C1-C2-C3	-2.80	106.10	109.65
3	C	603	FCA	O3-C3-C4	-2.67	104.55	110.36
4	C	605	MAN	C3-C4-C5	-2.38	106.03	110.22
4	C	604	MAN	C3-C4-C5	-2.12	106.48	110.22
3	C	603	FCA	O3-C3-C2	2.38	114.36	110.02
3	C	601	NAG	C3-C4-C5	2.76	115.08	110.22
4	C	605	MAN	O2-C2-C3	3.19	116.45	110.17
4	C	605	MAN	O5-C1-C2	3.34	116.02	110.79
3	C	601	NAG	C4-C3-C2	3.42	116.04	111.02
4	C	604	MAN	O5-C1-C2	3.47	116.23	110.79
3	C	603	FCA	C1-O5-C5	3.48	120.09	112.39
3	C	603	FCA	C1-C2-C3	3.63	114.26	109.65
3	C	601	NAG	O4-C4-C3	4.58	120.31	110.36
3	C	601	NAG	C6-C5-C4	5.28	125.36	113.00
3	C	601	NAG	O6-C6-C5	5.52	129.93	111.34
4	C	604	MAN	O2-C2-C3	6.12	122.19	110.17
3	C	601	NAG	O7-C7-C8	6.50	133.89	122.06
3	C	601	NAG	C1-O5-C5	7.10	121.95	112.17

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.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	601	NAG	3	0
3	C	603	FCA	2	0
4	C	604	MAN	2	0
4	C	605	MAN	2	0

5.6 Ligand geometry [i](#)

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	-	51,58,58	1.04	4 (7%)	54,89,89	2.58	14 (25%)
6	MD2	A	590	-	11,13,13	0.55	0	6,12,12	3.40	2 (33%)
2	NAG	A	601	1,2	14,14,15	1.71	3 (21%)	15,19,21	3.26	9 (60%)
2	NAG	A	602	2	14,14,15	1.49	2 (14%)	15,19,21	2.17	5 (33%)
5	FAD	B	579	-	51,58,58	0.97	2 (3%)	54,89,89	1.57	5 (9%)
6	MD2	B	590	-	11,13,13	0.59	0	6,12,12	1.43	1 (16%)
2	NAG	B	601	1,2	14,14,15	1.95	4 (28%)	15,19,21	3.05	10 (66%)
2	NAG	B	602	1,2	14,14,15	1.25	1 (7%)	15,19,21	2.94	6 (40%)
5	FAD	C	579	-	51,58,58	1.21	5 (9%)	54,89,89	2.43	8 (14%)
6	MD2	C	590	-	11,13,13	0.50	0	6,12,12	2.66	2 (33%)
2	NAG	C	602	3,4	14,14,15	1.53	3 (21%)	15,19,21	2.10	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	-	-	0/28/50/50	0/6/6/6
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	-	-	0/28/50/50	0/6/6/6
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
5	FAD	C	579	-	-	0/28/50/50	0/6/6/6
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 (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	602	NAG	C1-C2	-3.73	1.47	1.52
2	B	601	NAG	C1-C2	-3.41	1.47	1.52
5	C	579	FAD	C2-N1	-3.39	1.31	1.38
2	A	602	NAG	O5-C1	-3.06	1.38	1.43
5	A	579	FAD	C2-N1	-2.49	1.33	1.38
2	B	601	NAG	C4-C3	-2.27	1.46	1.52
2	C	602	NAG	O4-C4	-2.16	1.38	1.43
2	A	601	NAG	C1-C2	-2.11	1.49	1.52
5	B	579	FAD	C2-N1	-2.10	1.34	1.38
5	A	579	FAD	C4X-N5	2.01	1.36	1.33
5	A	579	FAD	C5'-C4'	2.03	1.54	1.51
5	C	579	FAD	C10-N1	2.12	1.36	1.33
5	C	579	FAD	C5'-C4'	2.18	1.55	1.51
2	B	602	NAG	C2-N2	2.32	1.50	1.46
2	B	601	NAG	O3-C3	2.63	1.49	1.43
2	C	602	NAG	O6-C6	2.76	1.54	1.42
5	C	579	FAD	C4X-N5	2.94	1.37	1.33
2	A	601	NAG	O3-C3	3.10	1.50	1.43
5	C	579	FAD	C4-N3	3.30	1.39	1.33
2	C	602	NAG	O5-C5	3.31	1.50	1.43
5	B	579	FAD	C4-N3	3.45	1.39	1.33
5	A	579	FAD	C4-N3	4.32	1.40	1.33
2	A	601	NAG	O5-C5	4.36	1.52	1.43
2	B	601	NAG	O5-C5	4.48	1.52	1.43

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	590	MD2	C11-N10-C9	-7.11	102.21	113.46
5	A	579	FAD	C4X-C10-N10	-7.04	115.63	120.52
5	C	579	FAD	C4X-C10-N10	-6.80	115.80	120.52
2	B	601	NAG	C2-N2-C7	-6.53	113.42	122.94
5	A	579	FAD	C4X-C4-N3	-6.32	114.48	123.48
2	A	602	NAG	C2-N2-C7	-6.09	114.05	122.94
5	C	579	FAD	C4X-C4-N3	-5.25	116.01	123.48
5	C	579	FAD	C4-C4X-C10	-4.98	115.93	119.96
5	B	579	FAD	C4X-C4-N3	-4.27	117.40	123.48
2	A	601	NAG	C8-C7-N2	-4.06	108.78	116.11
2	B	602	NAG	C2-N2-C7	-3.98	117.14	122.94
5	A	579	FAD	C9A-C5X-N5	-3.72	116.70	122.24
2	A	601	NAG	C2-N2-C7	-3.56	117.75	122.94
6	A	590	MD2	C8-C9-N10	-3.53	103.06	112.06
2	B	601	NAG	O4-C4-C5	-3.32	100.92	109.28
5	A	579	FAD	C4-C4X-C10	-3.18	117.39	119.96
2	A	601	NAG	O4-C4-C5	-3.09	101.50	109.28
2	B	601	NAG	O5-C1-C2	-2.77	107.62	111.47
5	C	579	FAD	O3'-C3'-C2'	-2.69	102.14	108.82
2	B	601	NAG	O4-C4-C3	-2.69	104.51	110.36
5	A	579	FAD	C1'-N10-C10	-2.44	116.00	118.50
5	A	579	FAD	O2'-C2'-C3'	-2.40	103.14	109.09
2	B	602	NAG	O5-C1-C2	-2.28	108.30	111.47
2	A	602	NAG	C8-C7-N2	-2.11	112.29	116.11
2	C	602	NAG	O5-C1-C2	-2.11	108.54	111.47
5	A	579	FAD	O2'-C2'-C1'	2.01	114.43	109.79
2	B	601	NAG	C6-C5-C4	2.01	117.70	113.00
5	A	579	FAD	O2A-PA-O1A	2.03	122.77	112.28
2	B	601	NAG	C3-C4-C5	2.09	113.90	110.22
5	A	579	FAD	C4X-N5-C5X	2.11	118.99	116.76
5	C	579	FAD	C4'-C3'-C2'	2.12	117.97	113.41
5	B	579	FAD	N6A-C6A-N1A	2.25	123.22	118.77
5	A	579	FAD	C2B-C3B-C4B	2.29	107.07	102.62
2	A	602	NAG	O4-C4-C5	2.32	115.13	109.28
2	A	602	NAG	C6-C5-C4	2.37	118.55	113.00
5	A	579	FAD	C6-C5X-C9A	2.38	122.08	119.00
2	B	601	NAG	O7-C7-C8	2.40	126.42	122.06
6	B	590	MD2	C7-C6-N5	2.41	118.21	112.06
2	A	601	NAG	C3-C4-C5	2.45	114.53	110.22
2	C	602	NAG	O3-C3-C4	2.47	115.73	110.36
5	A	579	FAD	C4A-C5A-N7A	2.49	111.82	109.41
2	A	602	NAG	O3-C3-C4	2.54	115.88	110.36
2	A	601	NAG	O3-C3-C4	2.66	116.15	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	590	MD2	C11-N10-C9	2.77	117.85	113.46
2	B	601	NAG	O3-C3-C4	2.78	116.40	110.36
5	C	579	FAD	C4-C4X-N5	2.89	121.85	118.68
2	B	602	NAG	O4-C4-C3	2.90	116.66	110.36
2	B	602	NAG	C1-O5-C5	3.19	116.56	112.17
2	A	601	NAG	O7-C7-C8	3.60	128.60	122.06
5	C	579	FAD	N3A-C2A-N1A	3.61	132.00	128.86
2	A	601	NAG	C6-C5-C4	3.76	121.80	113.00
5	B	579	FAD	C4A-C5A-N7A	3.76	113.05	109.41
2	B	602	NAG	C6-C5-C4	3.79	121.87	113.00
2	C	602	NAG	C1-O5-C5	4.23	118.00	112.17
5	B	579	FAD	C1'-N10-C9A	4.26	122.25	118.35
2	B	601	NAG	O6-C6-C5	4.65	126.98	111.34
2	B	601	NAG	C1-O5-C5	4.65	118.58	112.17
2	A	601	NAG	C1-O5-C5	4.85	118.86	112.17
2	C	602	NAG	O4-C4-C3	5.05	121.35	110.36
6	C	590	MD2	C4-N5-C6	5.51	122.18	113.46
5	B	579	FAD	C4-N3-C2	5.60	120.05	115.16
5	A	579	FAD	C1'-N10-C9A	6.59	124.39	118.35
2	A	601	NAG	O6-C6-C5	6.93	134.65	111.34
2	B	602	NAG	O6-C6-C5	8.23	139.05	111.34
5	A	579	FAD	C4-N3-C2	11.06	124.83	115.16
5	C	579	FAD	C4-N3-C2	11.86	125.53	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	579	FAD	2	0
6	A	590	MD2	4	0
2	A	601	NAG	3	0
2	A	602	NAG	3	0
6	B	590	MD2	5	0
2	B	601	NAG	4	0
2	B	602	NAG	4	0
6	C	590	MD2	6	0
2	C	602	NAG	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 [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	459/472 (97%)	-0.33	6 (1%) 77 80	6, 15, 38, 69	20 (4%)
1	B	462/472 (97%)	-0.41	7 (1%) 74 77	4, 13, 36, 70	18 (3%)
1	C	462/472 (97%)	-0.42	5 (1%) 80 83	5, 12, 36, 57	15 (3%)
All	All	1383/1416 (97%)	-0.39	18 (1%) 77 80	4, 13, 37, 70	53 (3%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	SER	3.5
1	A	50	ALA	3.4
1	A	379	GLY	3.4
1	A	341	ASP	2.9
1	B	463	CYS	2.7
1	C	223	SER	2.5
1	C	220	ASP	2.5
1	B	379	GLY	2.5
1	B	381	ASP	2.4
1	C	50	ALA	2.4
1	B	466	HIS	2.4
1	C	222	LYS	2.4
1	B	220	ASP	2.4
1	A	220	ASP	2.2
1	B	223	SER	2.2
1	C	254	ASN	2.2
1	A	222	LYS	2.0
1	B	462	MET	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 ⓘ

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	MAN	C	605	11/12	0.90	0.29	-	30,40,63,96	0
4	MAN	C	604	11/12	0.75	0.25	-	24,36,53,55	0
3	FCA	C	603	10/11	0.89	0.20	-	9,34,42,75	0
3	NAG	C	601	14/15	0.89	0.15	-	1,12,24,57	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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	MD2	B	590	14/14	0.93	0.16	6.58	13,33,55,55	0
6	MD2	C	590	14/14	0.91	0.14	5.52	19,30,38,46	0
6	MD2	A	590	14/14	0.93	0.14	3.90	19,32,39,41	0
2	NAG	B	601	14/15	0.87	0.15	1.84	9,24,38,100	0
5	FAD	B	579	53/53	0.98	0.07	-0.49	1,6,9,10	0
5	FAD	C	579	53/53	0.98	0.07	-0.84	3,7,12,12	0
5	FAD	A	579	53/53	0.98	0.07	-0.99	3,9,13,16	0
2	NAG	C	602	14/15	0.79	0.22	-	3,12,39,74	0
2	NAG	A	601	14/15	0.76	0.17	-	17,35,71,100	0
2	NAG	A	602	14/15	0.91	0.33	-	26,53,100,100	0
2	NAG	B	602	14/15	0.90	0.29	-	14,46,98,100	0

6.5 Other polymers ⓘ

There are no such residues in this entry.