



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:30 PM GMT

PDB ID : 1B37
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 : 1998-12-17
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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

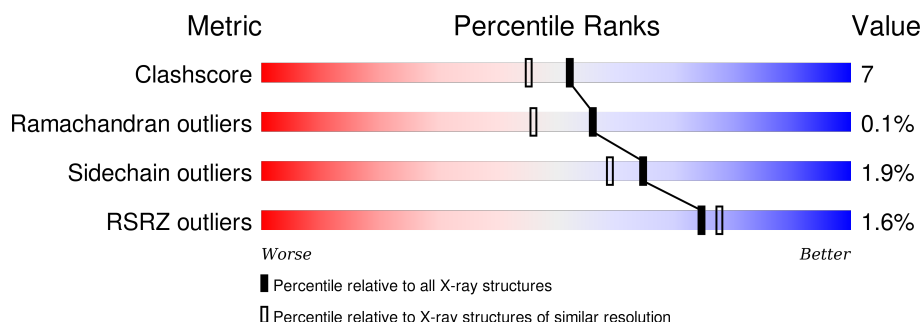
1 Overall quality at a glance

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	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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>2%</div> <div>77%</div> <div>18%</div> <div>..</div> </div>
1	B	472	<div> <div>2%</div> <div>83%</div> <div>13%</div> <div>..</div> </div>
1	C	472	<div> <div>%</div> <div>85%</div> <div>13%</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
2	NAG	A	850	-	-	-	X
4	MAN	C	604	X	-	-	-

2 Entry composition [i](#)

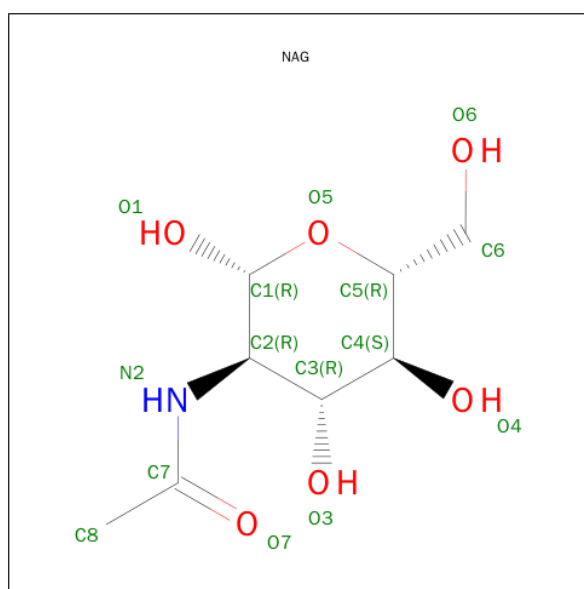
There are 6 unique types of molecules in this entry. The entry contains 12067 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	57	0	0
			3684	2353	621	696	14			
1	B	462	Total	C	N	O	S	59	0	0
			3715	2374	627	700	14			
1	C	462	Total	C	N	O	S	55	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	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		

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

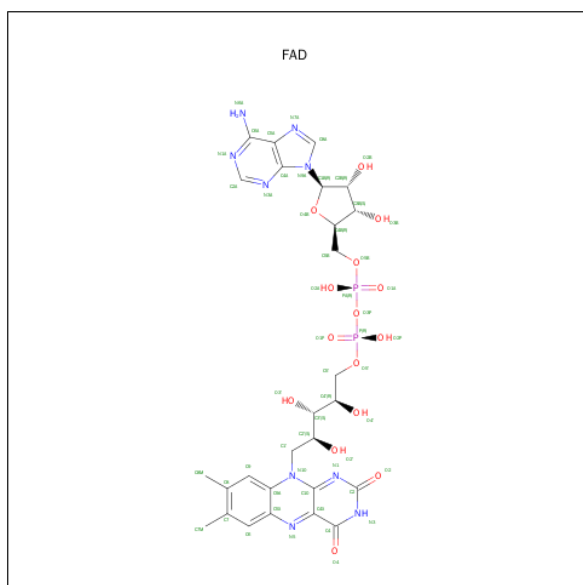
- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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 (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	3	Total	C	N	O	0	0
			36	20	1	15		

- 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		
5	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

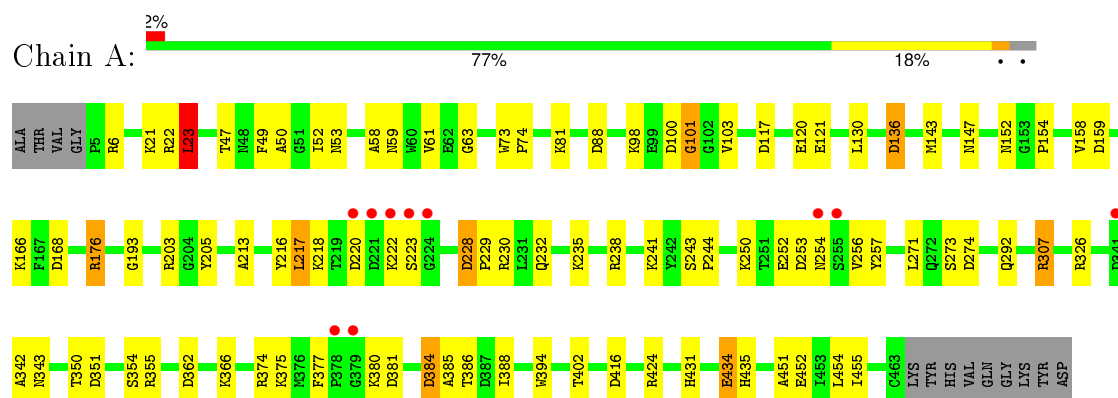
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	209	Total 209	O 209	0	0
6	B	220	Total 220	O 220	0	0
6	C	249	Total 249	O 249	0	0

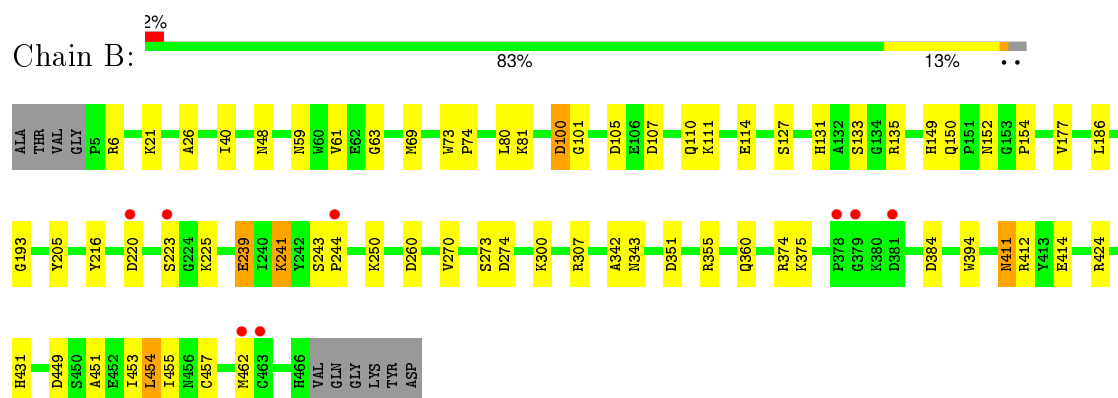
3 Residue-property plots [i](#)

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

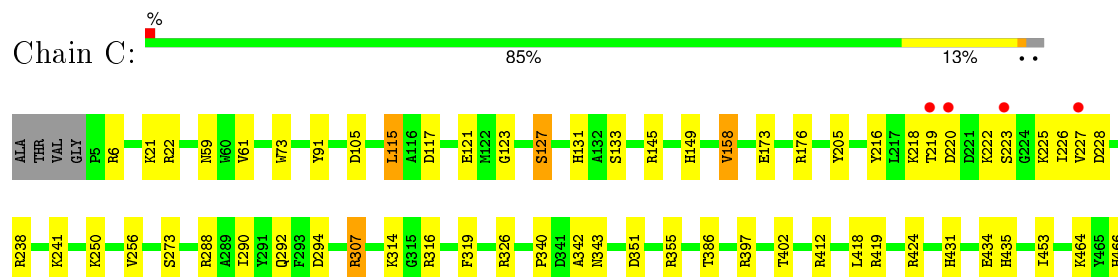
• Molecule 1: PROTEIN (POLYAMINE OXIDASE)



• Molecule 1: PROTEIN (POLYAMINE OXIDASE)



• Molecule 1: PROTEIN (POLYAMINE OXIDASE)



VAL
GLN
GLY
LYS
TYR
ASP

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	184.80Å 184.80Å 282.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.90 49.90 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.0 (50.00-1.90) 98.5 (49.90-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 1.91Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.199 , (Not available) 0.195 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 70.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 216246 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12067	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.75	0/3775	1.30	22/5116 (0.4%)
1	B	0.75	0/3808	1.26	18/5160 (0.3%)
1	C	0.76	0/3808	1.31	26/5160 (0.5%)
All	All	0.75	0/11391	1.29	66/15436 (0.4%)

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	C	1	0
4	C	1	0
All	All	2	0

There are no bond length outliers.

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	307	ARG	NE-CZ-NH1	-13.41	113.59	120.30
1	B	355	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	C	115	LEU	CB-CG-CD1	-9.61	94.67	111.00
1	C	424	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	A	101	GLY	N-CA-C	8.75	134.97	113.10
1	C	307	ARG	NE-CZ-NH2	8.73	124.67	120.30
1	A	355	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	C	176	ARG	NE-CZ-NH2	-7.21	116.70	120.30
1	C	397	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	A	23	LEU	CB-CG-CD1	6.95	122.82	111.00
1	B	186	LEU	CB-CG-CD2	-6.88	99.31	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	ARG	NE-CZ-NH1	-6.72	116.94	120.30
1	A	307	ARG	NE-CZ-NH1	-6.59	117.00	120.30
1	C	355	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	C	340	PRO	C-N-CA	-6.46	105.55	121.70
1	B	300	LYS	CD-CE-NZ	-6.42	96.94	111.70
1	A	136	ASP	CB-CA-C	-6.37	97.67	110.40
1	C	145	ARG	NE-CZ-NH1	-6.28	117.16	120.30
1	B	351	ASP	N-CA-CB	-6.28	99.29	110.60
1	C	307	ARG	CD-NE-CZ	-6.27	114.82	123.60
1	A	176	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	A	384	ASP	CB-CA-C	-6.09	98.23	110.40
1	B	454	LEU	CA-CB-CG	5.96	129.01	115.30
1	C	115	LEU	CB-CG-CD2	-5.92	100.94	111.00
1	A	61	VAL	N-CA-C	-5.91	95.05	111.00
1	A	351	ASP	N-CA-CB	-5.84	100.08	110.60
1	B	6	ARG	NE-CZ-NH1	-5.75	117.42	120.30
1	A	88	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	424	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	C	238	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	307	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	374	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	C	61	VAL	N-CA-C	-5.55	96.03	111.00
1	C	241	LYS	CD-CE-NZ	5.54	124.44	111.70
1	C	176	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	61	VAL	N-CA-C	-5.49	96.18	111.00
1	C	412	ARG	NE-CZ-NH1	-5.48	117.56	120.30
1	C	22	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	228	ASP	CB-CG-OD2	-5.47	113.37	118.30
1	C	419	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	C	273	SER	C-N-CA	-5.40	108.19	121.70
1	B	135	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	A	454	LEU	CB-CG-CD1	-5.38	101.86	111.00
1	A	22	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	412	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	A	362	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	271	LEU	CB-CG-CD1	-5.35	101.91	111.00
1	A	230	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	374	ARG	NE-CZ-NH2	5.31	122.95	120.30
1	C	326	ARG	NE-CZ-NH1	-5.25	117.68	120.30
1	A	416	ASP	CB-CG-OD2	-5.24	113.59	118.30
1	C	351	ASP	N-CA-CB	-5.21	101.21	110.60
1	C	22	ARG	NE-CZ-NH2	-5.21	117.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	ARG	NE-CZ-NH1	-5.21	117.70	120.30
1	C	316	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	B	101	GLY	N-CA-C	5.20	126.09	113.10
1	B	149	HIS	CB-CA-C	-5.17	100.06	110.40
1	C	158	VAL	CG1-CB-CG2	-5.17	102.63	110.90
1	B	384	ASP	CB-CG-OD1	5.15	122.94	118.30
1	B	239	GLU	OE1-CD-OE2	-5.09	117.19	123.30
1	B	270	VAL	CG1-CB-CG2	-5.09	102.76	110.90
1	C	288	ARG	NE-CZ-NH1	-5.09	117.76	120.30
1	B	241	LYS	CD-CE-NZ	5.05	123.32	111.70
1	B	100	ASP	CB-CA-C	5.05	120.49	110.40
1	C	397	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	A	381	ASP	N-CA-C	-5.03	97.43	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	386	THR	CB
4	C	604	MAN	C1

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3584	55	0
1	B	3715	0	3614	54	1
1	C	3715	0	3613	38	0
2	A	28	0	25	0	0
2	B	28	0	25	0	1
3	C	24	0	22	4	0
4	C	36	0	30	2	0
5	A	53	0	31	3	0
5	B	53	0	31	0	0
5	C	53	0	31	2	0
6	A	209	0	0	2	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	220	0	0	3	1
6	C	249	0	0	4	3
All	All	12067	0	11006	145	4

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 (145) 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:B:69:MET:HE2	1:B:74:PRO:HD3	1.41	1.03
1:B:69:MET:CE	1:B:73:TRP:HB3	1.94	0.97
1:C:91:TYR:OH	1:C:314:LYS:HE2	1.70	0.92
1:B:69:MET:CE	1:B:74:PRO:HD3	2.01	0.90
1:C:131:HIS:CD2	1:C:133:SER:H	1.89	0.89
3:C:601:NAG:C4	4:C:602:NAG:C1	2.51	0.89
1:B:69:MET:HE3	1:B:73:TRP:HB3	1.56	0.84
1:A:273:SER:O	1:A:274:ASP:HB2	1.77	0.83
1:B:411:ASN:ND2	1:B:414:GLU:H	1.85	0.75
1:C:292:GLN:OE1	6:C:1019:HOH:O	2.02	0.75
1:A:431:HIS:H	1:A:431:HIS:CD2	2.03	0.75
1:B:131:HIS:CD2	1:B:133:SER:H	2.05	0.74
1:B:131:HIS:HD2	1:B:133:SER:H	1.37	0.72
1:C:131:HIS:HD2	1:C:133:SER:H	1.34	0.72
1:B:114:GLU:OE1	1:B:114:GLU:HA	1.91	0.71
1:C:117:ASP:O	1:C:121:GLU:HG3	1.91	0.70
1:B:220:ASP:HB3	1:B:223:SER:OG	1.92	0.70
1:A:130:LEU:HD22	1:A:136:ASP:HB2	1.76	0.68
1:A:434:GLU:HG2	1:A:435:HIS:CD2	2.31	0.65
1:A:394:TRP:HE1	1:B:152:ASN:ND2	1.93	0.65
1:B:411:ASN:HD22	1:B:414:GLU:H	1.45	0.65
1:A:73:TRP:HB3	1:A:74:PRO:HD3	1.81	0.63
1:A:216:TYR:CD1	1:A:217:LEU:HD13	2.33	0.63
1:A:229:PRO:O	1:A:232:GLN:NE2	2.32	0.62
1:C:220:ASP:HB3	1:C:223:SER:OG	2.00	0.62
1:B:431:HIS:CD2	1:B:431:HIS:H	2.18	0.61
1:C:220:ASP:OD2	1:C:222:LYS:N	2.35	0.60
3:C:601:NAG:H4	4:C:602:NAG:C1	2.33	0.58
1:B:241:LYS:HE3	1:B:250:LYS:HE3	1.84	0.58
1:C:431:HIS:H	1:C:431:HIS:CD2	2.19	0.58
1:B:243:SER:HB2	1:B:244:PRO:CD	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:LYS:HD2	1:A:385:ALA:HB3	1.86	0.57
1:C:131:HIS:HD2	1:C:133:SER:OG	1.87	0.57
1:C:250:LYS:HG2	1:C:256:VAL:HG22	1.86	0.57
1:A:216:TYR:CE1	1:A:217:LEU:HD13	2.41	0.56
1:B:243:SER:HB2	1:B:244:PRO:HD2	1.88	0.56
1:B:81:LYS:NZ	1:B:81:LYS:HB3	2.21	0.55
1:A:220:ASP:HB3	1:A:223:SER:OG	2.08	0.54
1:A:292:GLN:OE1	6:A:1029:HOH:O	2.19	0.53
1:B:457:CYS:HA	1:B:462:MET:O	2.09	0.53
1:C:342:ALA:O	1:C:343:ASN:HB2	2.09	0.53
1:B:449:ASP:O	1:B:453:ILE:HG13	2.08	0.52
1:C:131:HIS:CD2	1:C:133:SER:OG	2.62	0.52
1:C:91:TYR:HH	1:C:314:LYS:HE2	1.72	0.52
1:C:131:HIS:HD2	1:C:133:SER:CB	2.23	0.52
1:A:394:TRP:HE1	1:B:152:ASN:HD22	1.57	0.51
1:C:219:THR:HG22	1:C:226:ILE:HA	1.93	0.51
1:A:152:ASN:ND2	1:B:394:TRP:HE1	2.08	0.51
1:B:69:MET:HE2	1:B:73:TRP:HB3	1.85	0.51
1:C:464:LYS:HG2	1:C:466:HIS:O	2.10	0.51
1:B:451:ALA:O	1:B:455:ILE:HG13	2.11	0.51
1:A:58:ALA:HA	5:A:800:FAD:C4X	2.41	0.51
1:B:100:ASP:OD2	1:B:375:LYS:NZ	2.43	0.51
1:C:131:HIS:HD2	1:C:133:SER:N	2.07	0.51
1:A:63:GLY:HA2	1:A:193:GLY:O	2.11	0.51
1:B:273:SER:O	1:B:274:ASP:HB2	2.11	0.50
1:A:218:LYS:H	1:A:228:ASP:HB2	1.77	0.50
1:B:131:HIS:HD2	1:B:133:SER:OG	1.95	0.50
1:A:220:ASP:OD1	1:A:222:LYS:N	2.44	0.50
1:A:243:SER:HB2	1:A:244:PRO:CD	2.40	0.50
1:B:360:GLN:NE2	6:B:934:HOH:O	2.44	0.50
1:A:23:LEU:HD13	1:A:451:ALA:HB1	1.93	0.49
1:B:114:GLU:OE1	6:B:1063:HOH:O	2.19	0.49
1:B:80:LEU:O	1:B:81:LYS:HB2	2.12	0.49
1:A:241:LYS:HE3	1:A:250:LYS:HE3	1.95	0.49
1:A:431:HIS:CD2	6:A:880:HOH:O	2.65	0.49
1:A:120:GLU:OE1	1:A:166:LYS:NZ	2.32	0.49
1:A:49:PHE:O	1:A:50:ALA:HB3	2.12	0.48
1:B:69:MET:HE3	1:B:73:TRP:CD1	2.48	0.48
1:A:152:ASN:HD22	1:B:394:TRP:HE1	1.59	0.48
1:C:218:LYS:H	1:C:228:ASP:HB2	1.79	0.48
1:C:402:THR:CB	5:C:802:FAD:HM83	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:ASN:HD21	1:B:414:GLU:HG3	1.79	0.48
1:B:69:MET:HE3	1:B:73:TRP:CB	2.37	0.48
1:C:307:ARG:NH1	6:C:957:HOH:O	2.28	0.48
1:B:131:HIS:CD2	1:B:133:SER:OG	2.67	0.47
1:C:218:LYS:O	1:C:227:VAL:N	2.39	0.47
1:B:342:ALA:O	1:B:343:ASN:HB2	2.15	0.47
1:C:219:THR:HA	1:C:225:LYS:O	2.14	0.46
1:A:273:SER:O	1:A:274:ASP:CB	2.42	0.46
1:B:69:MET:HE1	1:B:74:PRO:HD3	1.92	0.46
1:C:131:HIS:CD2	1:C:133:SER:CB	2.99	0.46
1:A:434:GLU:O	1:A:434:GLU:HG3	2.14	0.46
1:C:220:ASP:OD2	1:C:222:LYS:HB3	2.15	0.46
1:C:402:THR:HB	5:C:802:FAD:HM83	1.98	0.46
1:A:402:THR:HB	5:A:800:FAD:HM83	1.97	0.46
1:B:69:MET:CE	1:B:73:TRP:CD1	2.99	0.45
1:A:143:MET:SD	1:A:147:ASN:ND2	2.90	0.45
1:A:434:GLU:HG2	1:A:435:HIS:NE2	2.31	0.45
1:A:213:ALA:O	1:A:217:LEU:HB2	2.17	0.45
1:B:63:GLY:HA2	1:B:193:GLY:O	2.16	0.45
1:B:131:HIS:HD2	1:B:133:SER:CB	2.30	0.45
1:A:307:ARG:HG2	1:A:307:ARG:NH1	2.31	0.45
1:A:81:LYS:O	1:A:203:ARG:NH2	2.50	0.45
1:A:388:ILE:HG21	1:A:388:ILE:HD13	1.74	0.45
1:C:173:GLU:OE1	1:C:294:ASP:OD2	2.35	0.44
1:A:176:ARG:HD2	1:B:177:VAL:HG21	1.98	0.44
1:B:150:GLN:NE2	6:B:932:HOH:O	2.50	0.44
1:A:238:ARG:NH1	1:A:252:GLU:OE2	2.48	0.44
1:A:73:TRP:N	1:A:74:PRO:CD	2.81	0.44
1:B:114:GLU:CA	1:B:114:GLU:OE1	2.61	0.44
1:B:107:ASP:O	1:B:111:LYS:HG3	2.18	0.44
1:A:307:ARG:HG2	1:A:307:ARG:HH11	1.83	0.43
1:C:453:ILE:HA	1:C:453:ILE:HD13	1.62	0.43
1:B:69:MET:CE	1:B:73:TRP:HD1	2.30	0.43
1:A:402:THR:CB	5:A:800:FAD:HM83	2.49	0.43
1:C:158:VAL:HG12	6:C:995:HOH:O	2.17	0.43
1:B:110:GLN:O	1:B:114:GLU:HG2	2.17	0.43
1:A:243:SER:CB	1:A:244:PRO:CD	2.97	0.43
1:A:47:THR:O	1:A:53:ASN:HA	2.19	0.43
1:B:411:ASN:C	1:B:411:ASN:HD22	2.22	0.43
3:C:601:NAG:H3	3:C:603:FCA:O2	2.18	0.43
1:C:6:ARG:HH11	1:C:6:ARG:HG3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:ILE:HA	1:C:418:LEU:HD21	2.01	0.42
1:C:431:HIS:CD2	6:C:810:HOH:O	2.72	0.42
1:A:98:LYS:HE3	1:A:103:VAL:O	2.18	0.42
1:B:81:LYS:NZ	1:B:81:LYS:CB	2.82	0.42
1:A:350:THR:HA	1:A:354:SER:OG	2.19	0.42
1:C:21:LYS:HB2	1:C:216:TYR:CE2	2.55	0.42
1:B:243:SER:CB	1:B:244:PRO:CD	2.95	0.42
1:A:256:VAL:HG12	1:A:257:TYR:N	2.35	0.42
1:B:223:SER:HB2	1:B:225:LYS:HG3	2.00	0.42
1:B:26:ALA:HB2	1:B:455:ILE:HD13	2.02	0.42
1:A:342:ALA:O	1:A:343:ASN:HB2	2.21	0.41
1:B:220:ASP:CB	1:B:223:SER:OG	2.64	0.41
1:B:239:GLU:OE2	1:B:241:LYS:HE2	2.20	0.41
1:A:235:LYS:NZ	1:A:253:ASP:OD2	2.38	0.41
1:B:40:ILE:HD13	1:B:40:ILE:HG21	1.66	0.41
1:A:253:ASP:O	1:A:254:ASN:HB2	2.20	0.41
1:B:21:LYS:HB2	1:B:216:TYR:CE2	2.55	0.41
1:C:73:TRP:HE1	3:C:601:NAG:C7	2.34	0.41
1:A:49:PHE:N	1:A:52:ILE:O	2.38	0.41
1:C:218:LYS:N	1:C:228:ASP:HB2	2.36	0.41
1:A:158:VAL:HG13	1:A:159:ASP:N	2.36	0.41
1:A:377:PHE:HB3	1:A:380:LYS:HG2	2.03	0.41
1:A:452:GLU:HA	1:A:455:ILE:HD12	2.02	0.40
1:A:117:ASP:O	1:A:121:GLU:HG3	2.21	0.40
1:A:100:ASP:OD1	1:A:375:LYS:HE2	2.21	0.40
1:C:386:THR:HG22	1:C:386:THR:H	1.62	0.40
1:A:217:LEU:HD12	1:A:217:LEU:HA	1.77	0.40
1:A:21:LYS:HB2	1:A:216:TYR:CE2	2.56	0.40
1:C:418:LEU:HA	1:C:418:LEU:HD23	1.93	0.40
1:C:434:GLU:CG	1:C:435:HIS:CD2	3.04	0.40
1:C:123:GLY:O	1:C:127:SER:HB2	2.21	0.40
1:B:260:ASP:O	1:B:424:ARG:HD3	2.21	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:928:HOH:O	6:C:928:HOH:O[10_665]	0.94	1.26
6:B:943:HOH:O	6:C:1014:HOH:O[10_665]	1.82	0.38
6:A:1038:HOH:O	6:C:1017:HOH:O[8_665]	2.16	0.04
1:B:48:ASN:ND2	2:B:853:NAG:C8[9_765]	2.18	0.02

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	457/472 (97%)	438 (96%)	18 (4%)	1 (0%)	52	42
1	B	460/472 (98%)	442 (96%)	18 (4%)	0	100	100
1	C	460/472 (98%)	443 (96%)	17 (4%)	0	100	100
All	All	1377/1416 (97%)	1323 (96%)	53 (4%)	1 (0%)	56	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	GLY

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	394/404 (98%)	385 (98%)	9 (2%)	58	51
1	B	397/404 (98%)	390 (98%)	7 (2%)	66	61
1	C	397/404 (98%)	390 (98%)	7 (2%)	66	61
All	All	1188/1212 (98%)	1165 (98%)	23 (2%)	65	59

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	59	ASN

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Mol	Chain	Res	Type
1	A	154	PRO
1	A	168	ASP
1	A	205	TYR
1	A	217	LEU
1	A	384	ASP
1	A	386	THR
1	A	434	GLU
1	B	59	ASN
1	B	105	ASP
1	B	127	SER
1	B	154	PRO
1	B	205	TYR
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	205	TYR
1	C	319	PHE

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

Mol	Chain	Res	Type
1	A	48	ASN
1	A	152	ASN
1	A	360	GLN
1	A	431	HIS
1	B	131	HIS
1	B	149	HIS
1	B	150	GLN
1	B	152	ASN
1	B	360	GLN
1	B	411	ASN
1	B	431	HIS
1	B	466	HIS
1	C	48	ASN
1	C	131	HIS
1	C	152	ASN
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 ⓘ

5 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	1,3,4	14,14,15	1.55	2 (14%)	15,19,21	4.17	9 (60%)
4	NAG	C	602	3,4	14,14,15	1.00	1 (7%)	15,19,21	1.73	4 (26%)
3	FCA	C	603	3	10,10,11	1.31	1 (10%)	14,14,16	2.72	7 (50%)
4	MAN	C	604	4	11,11,12	0.88	0	14,15,17	3.44	2 (14%)
4	MAN	C	605	4	11,11,12	0.73	0	14,15,17	1.48	3 (21%)

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	1,3,4	-	0/6/23/26	0/1/1/1
4	NAG	C	602	3,4	-	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	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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	NAG	C1-C2	-3.98	1.46	1.52
3	C	601	NAG	O5-C1	-3.74	1.37	1.43
3	C	603	FCA	C2-C3	-3.01	1.48	1.52
4	C	602	NAG	O5-C1	-2.95	1.38	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	NAG	C8-C7-N2	-8.83	99.21	116.11
3	C	601	NAG	O5-C5-C6	-7.08	92.02	107.35
4	C	604	MAN	O2-C2-C1	-4.84	99.50	109.21
3	C	603	FCA	O5-C5-C6	-4.77	98.24	106.13
3	C	603	FCA	O5-C1-C2	-4.38	103.75	110.86
3	C	603	FCA	C3-C4-C5	-3.36	104.05	109.72
4	C	602	NAG	O5-C5-C6	-3.30	100.20	107.35
4	C	605	MAN	C3-C4-C5	-2.97	105.02	110.20
4	C	605	MAN	C1-C2-C3	-2.85	106.17	109.54
3	C	601	NAG	C3-C4-C5	-2.47	105.90	110.20
4	C	602	NAG	O4-C4-C5	-2.37	102.96	109.24
3	C	603	FCA	O3-C3-C4	-2.30	105.16	110.34
3	C	603	FCA	O2-C2-C3	-2.25	105.59	110.12
3	C	601	NAG	C6-C5-C4	2.03	118.03	113.02
4	C	605	MAN	O2-C2-C1	2.08	113.37	109.21
4	C	602	NAG	O3-C3-C4	2.17	115.23	110.34
3	C	601	NAG	C4-C3-C2	2.46	115.05	111.23
3	C	601	NAG	O6-C6-C5	2.86	120.78	111.33
3	C	601	NAG	O7-C7-N2	3.20	128.40	121.86
4	C	602	NAG	C1-O5-C5	3.78	117.04	112.25
3	C	603	FCA	C1-C2-C3	3.79	114.03	109.54
3	C	603	FCA	C1-O5-C5	4.36	119.11	112.38
3	C	601	NAG	O7-C7-C8	5.60	132.34	122.06
3	C	601	NAG	C1-O5-C5	7.83	122.18	112.25
4	C	604	MAN	O2-C2-C3	11.20	132.64	110.12

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.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	601	NAG	4	0
4	C	602	NAG	2	0
3	C	603	FCA	1	0

5.6 Ligand geometry

7 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	800	-	48,58,58	1.16	3 (6%)	54,89,89	2.38	9 (16%)
2	NAG	A	850	1,2	14,14,15	1.33	1 (7%)	15,19,21	3.13	4 (26%)
2	NAG	A	851	2	14,14,15	0.81	0	15,19,21	3.09	4 (26%)
5	FAD	B	801	-	48,58,58	0.96	2 (4%)	54,89,89	1.83	8 (14%)
2	NAG	B	852	1,2	14,14,15	1.44	2 (14%)	15,19,21	2.51	6 (40%)
2	NAG	B	853	2	14,14,15	1.47	3 (21%)	15,19,21	3.38	6 (40%)
5	FAD	C	802	-	48,58,58	1.16	3 (6%)	54,89,89	2.47	8 (14%)

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	800	-	-	0/30/50/50	0/6/6/6
2	NAG	A	850	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	851	2	-	0/6/23/26	0/1/1/1
5	FAD	B	801	-	-	0/30/50/50	0/6/6/6
2	NAG	B	852	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	853	2	-	0/6/23/26	0/1/1/1
5	FAD	C	802	-	-	0/30/50/50	0/6/6/6

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	852	NAG	C1-C2	-4.12	1.46	1.52
2	B	853	NAG	O5-C1	-3.55	1.37	1.43
2	A	850	NAG	O5-C1	-3.44	1.38	1.43
5	A	800	FAD	C10-N10	-3.21	1.35	1.39
2	B	852	NAG	O5-C1	-2.26	1.39	1.43
2	B	853	NAG	C6-C5	-2.05	1.44	1.51
5	A	800	FAD	C5'-C4'	2.09	1.54	1.51
2	B	853	NAG	C4-C5	2.09	1.57	1.53
5	C	802	FAD	C5'-C4'	2.24	1.55	1.51
5	B	801	FAD	C4X-N5	2.48	1.37	1.33
5	C	802	FAD	C4-N3	3.39	1.39	1.33
5	C	802	FAD	C4X-N5	3.50	1.38	1.33
5	B	801	FAD	C4-N3	3.60	1.39	1.33
5	A	800	FAD	C4-N3	4.73	1.41	1.33

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	802	FAD	C4X-C10-N10	-10.15	114.54	120.52
2	A	851	NAG	C2-N2-C7	-8.47	112.16	123.04
5	A	800	FAD	C4X-C10-N10	-8.14	115.72	120.52
5	A	800	FAD	C4X-C4-N3	-6.71	114.41	123.59
2	A	850	NAG	O5-C5-C6	-6.46	93.36	107.35
5	C	802	FAD	C4-C4X-C10	-5.38	116.50	119.94
5	C	802	FAD	C4X-C4-N3	-4.86	116.94	123.59
5	B	801	FAD	C4X-C4-N3	-4.83	116.98	123.59
5	A	800	FAD	C9A-C5X-N5	-4.09	116.30	122.36
2	B	853	NAG	C2-N2-C7	-4.02	117.87	123.04
2	B	852	NAG	O5-C5-C6	-3.63	99.50	107.35
2	A	850	NAG	O4-C4-C5	-3.17	100.84	109.24
5	B	801	FAD	C4X-C10-N10	-3.15	118.66	120.52
5	B	801	FAD	O3'-C3'-C4'	-2.46	102.56	108.75
2	B	852	NAG	C2-N2-C7	-2.41	119.94	123.04
5	B	801	FAD	C4-C4X-C10	-2.31	118.46	119.94
5	C	802	FAD	P-O3P-PA	-2.03	127.04	132.73
2	B	852	NAG	C8-C7-N2	-2.02	112.25	116.11
2	B	853	NAG	O4-C4-C5	2.10	114.80	109.24
5	A	800	FAD	C5X-C9A-N10	2.14	119.25	117.62
2	B	852	NAG	C6-C5-C4	2.17	118.37	113.02
5	C	802	FAD	C4-C4X-N5	2.18	121.36	118.72
5	B	801	FAD	C7M-C7-C8	2.20	125.57	120.73
5	B	801	FAD	C1'-N10-C9A	2.25	121.38	118.86
2	B	852	NAG	O6-C6-C5	2.27	118.82	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	800	FAD	O4'-C4'-C3'	2.27	114.72	109.02
2	B	853	NAG	O6-C6-C5	2.32	119.00	111.33
2	B	853	NAG	C6-C5-C4	2.36	118.83	113.02
2	A	851	NAG	O5-C5-C6	2.38	112.50	107.35
5	A	800	FAD	C4X-N5-C5X	2.47	119.61	116.76
5	C	802	FAD	C4A-C5A-N7A	2.60	111.87	109.48
2	B	853	NAG	C3-C2-N2	2.77	117.19	110.56
5	B	801	FAD	C4-C4X-N5	3.22	122.63	118.72
2	A	851	NAG	C6-C5-C4	3.23	120.99	113.02
5	A	800	FAD	C6-C5X-C9A	3.24	123.24	118.98
5	C	802	FAD	N3A-C2A-N1A	3.71	131.74	128.89
5	A	800	FAD	C1'-N10-C9A	4.52	123.94	118.86
2	A	850	NAG	C6-C5-C4	5.13	125.66	113.02
2	A	851	NAG	C1-O5-C5	6.34	120.29	112.25
2	A	850	NAG	C1-O5-C5	7.30	121.51	112.25
2	B	852	NAG	C1-O5-C5	7.34	121.56	112.25
5	B	801	FAD	C4-N3-C2	8.14	122.28	115.25
5	A	800	FAD	C4-N3-C2	9.67	123.60	115.25
5	C	802	FAD	C4-N3-C2	10.27	124.13	115.25
2	B	853	NAG	C1-O5-C5	11.39	126.70	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	800	FAD	3	0
2	B	853	NAG	0	1
5	C	802	FAD	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	459/472 (97%)	-0.03	10 (2%) 65 68	4, 14, 36, 61	19 (4%)
1	B	462/472 (97%)	-0.12	8 (1%) 73 76	3, 12, 33, 67	20 (4%)
1	C	462/472 (97%)	-0.22	4 (0%) 85 87	3, 11, 31, 51	19 (4%)
All	All	1383/1416 (97%)	-0.12	22 (1%) 74 78	3, 12, 34, 67	58 (4%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	SER	4.0
1	B	379	GLY	3.8
1	B	381	ASP	3.5
1	A	379	GLY	3.4
1	A	341	ASP	3.2
1	C	223	SER	3.1
1	B	220	ASP	2.9
1	A	222	LYS	2.8
1	C	227	VAL	2.8
1	A	254	ASN	2.7
1	A	221	ASP	2.6
1	B	223	SER	2.5
1	A	220	ASP	2.5
1	A	378	PRO	2.4
1	A	255	SER	2.3
1	B	244	PRO	2.3
1	C	220	ASP	2.3
1	B	462	MET	2.2
1	C	219	THR	2.2
1	B	463	CYS	2.1
1	B	378	PRO	2.1
1	A	224	GLY	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](#)

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
3	FCA	C	603	10/11	0.83	0.21	-	6,30,36,100	0
4	MAN	C	605	11/12	0.89	0.23	-	31,44,73,100	0
3	NAG	C	601	14/15	0.80	0.17	-	5,15,34,100	0
4	MAN	C	604	11/12	0.70	0.21	-	25,43,66,74	0
4	NAG	C	602	14/15	0.82	0.19	-	5,17,31,65	0

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. 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
2	NAG	A	850	14/15	0.78	0.20	2.10	23,35,59,59	0
5	FAD	C	802	53/53	0.97	0.09	-0.41	1,7,11,11	0
5	FAD	A	800	53/53	0.97	0.08	-0.68	3,8,12,14	0
5	FAD	B	801	53/53	0.98	0.08	-0.71	1,6,8,9	0
2	NAG	A	851	14/15	0.85	0.33	-	22,45,94,100	0
2	NAG	B	852	14/15	0.85	0.17	-	13,29,38,100	0
2	NAG	B	853	14/15	0.87	0.19	-	18,52,100,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.