



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:23 pm GMT

PDB ID : 3GDN
Title : Almond hydroxynitrile lyase in complex with benzaldehyde
Authors : Dreveny, I.; Gruber, K.; Kratky, C.
Deposited on : 2009-02-24
Resolution : 1.67 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

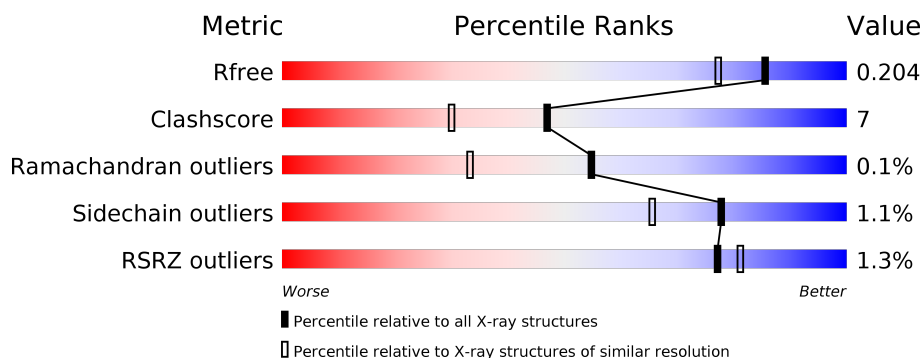
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.67 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	5252 (1.70-1.66)
Clashscore	112137	5803 (1.70-1.66)
Ramachandran outliers	110173	5704 (1.70-1.66)
Sidechain outliers	110143	5703 (1.70-1.66)
RSRZ outliers	101464	5298 (1.70-1.66)

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	521	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>15%</div> </div> </div>
1	B	521	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>14%</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
5	NAG	A	527	-	-	-	X
7	MXN	A	531	-	-	-	X
7	MXN	A	532	-	-	-	X
7	MXN	B	534	-	-	-	X
7	MXN	B	535	-	-	-	X
9	NAG	B	528	-	-	-	X

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 9681 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.

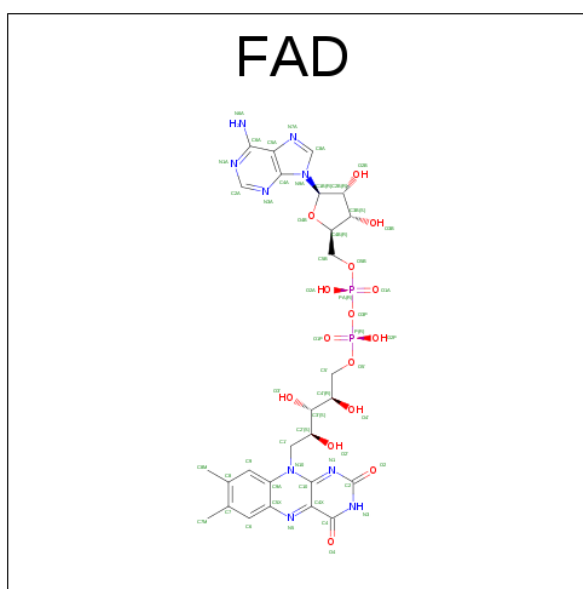
- Molecule 1 is a protein called R-oxynitrile lyase isoenzyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	521	Total	C	N	O	S	0	8	0
			4016	2552	668	788	8			
1	B	521	Total	C	N	O	S	0	9	0
			4019	2553	669	789	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	346	SER	ALA	SEE REMARK 999	UNP Q945K2
B	346	SER	ALA	SEE REMARK 999	UNP Q945K2

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



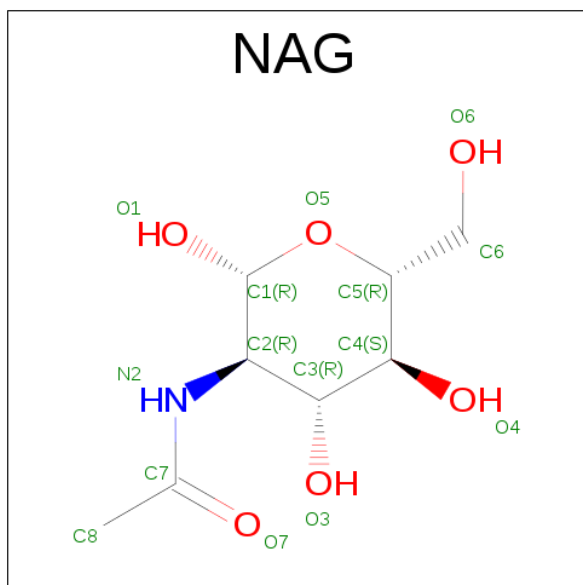
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

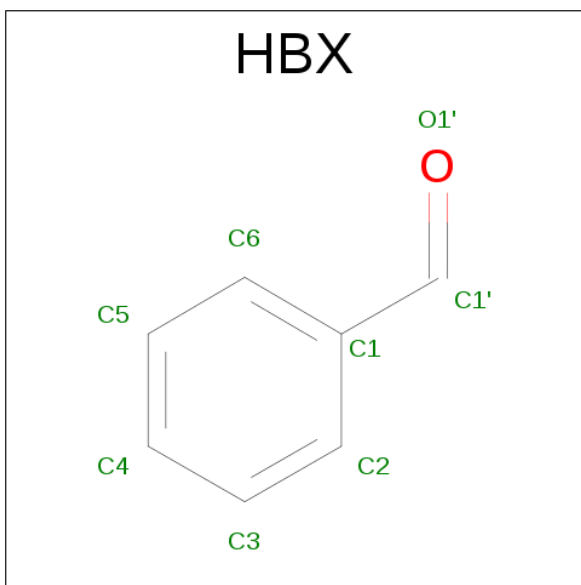
- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

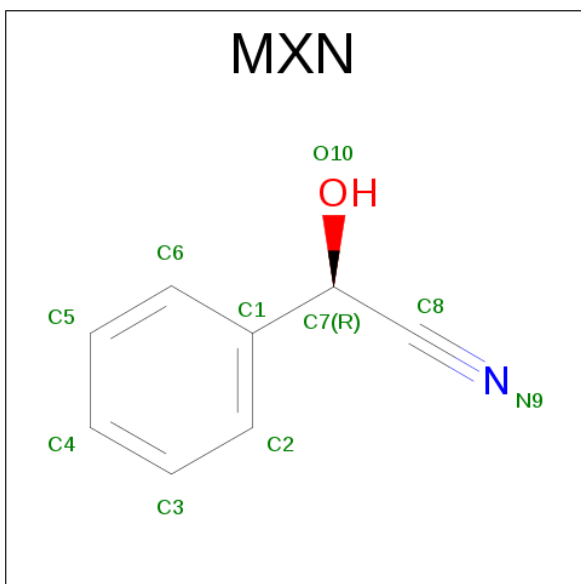
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 6 is BENZALDEHYDE (three-letter code: HBX) (formula: C_7H_6O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	7	1		
6	B	1	Total	C	O	0	0
			8	7	1		

- Molecule 7 is (2R)-HYDROXY(PHENYL)ETHANENITRILE (three-letter code: MXN) (formula: C₈H₇NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			10	8	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			10	8	1	1		
7	B	1	Total	C	N	O	0	0
			10	8	1	1		
7	B	1	Total	C	N	O	0	0
			10	8	1	1		

- Molecule 8 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	5	Total	C	N	O	0	0
			60	34	2	24		

- Molecule 9 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	4	Total	C	N	O	0	0
			50	28	2	20		

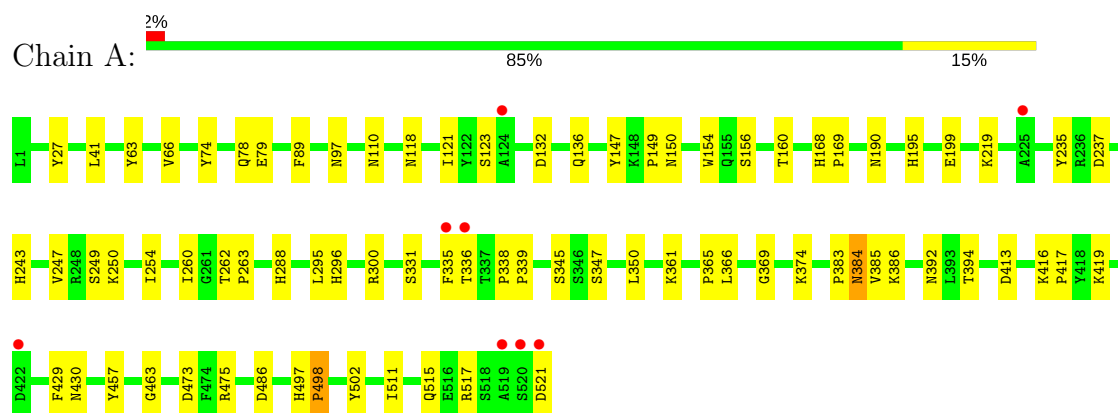
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	643	Total	O	0	0
			643	643		
10	B	626	Total	O	0	0
			626	626		

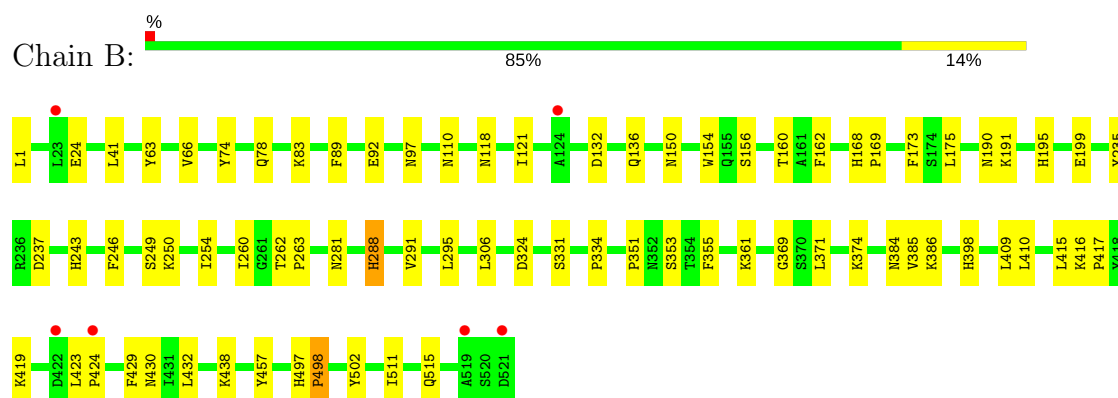
3 Residue-property plots [i](#)

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: R-oxynitrile lyase isoenzyme 1



• Molecule 1: R-oxynitrile lyase isoenzyme 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.98Å 93.79Å 86.90Å 90.00° 106.47° 90.00°	Depositor
Resolution (Å)	19.97 – 1.67 19.96 – 1.67	Depositor EDS
% Data completeness (in resolution range)	86.3 (19.97-1.67) 86.3 (19.96-1.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.30 (at 1.67Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.174 , 0.197 0.183 , 0.204	Depositor DCC
R_{free} test set	10601 reflections (10.00%)	DCC
Wilson B-factor (Å ²)	13.5	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9681	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.14 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.0353e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MXN, FUC, MAN, FAD, HBX

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	0.35	2/4162 (0.0%)	0.63	0/5677
1	B	0.30	0/4170	0.63	0/5688
All	All	0.32	2/8332 (0.0%)	0.63	0/11365

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	384[A]	ASN	CB-CG	-8.21	1.32	1.51
1	A	384[B]	ASN	CB-CG	-8.21	1.32	1.51

There are no bond angle outliers.

There are no chirality outliers.

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	4016	0	3882	58	0
1	B	4019	0	3884	55	0
2	A	53	0	31	3	0
2	B	53	0	31	3	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	A	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	38	0	34	2	0
6	A	8	0	6	0	0
6	B	8	0	6	0	0
7	A	20	0	14	1	0
7	B	20	0	14	1	0
8	B	60	0	52	3	0
9	B	50	0	43	0	0
10	A	643	0	0	5	0
10	B	626	0	0	6	0
All	All	9681	0	8057	117	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 (117) 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:150:ASN:ND2	1:A:190:ASN:HD22	1.60	0.99
1:B:295:LEU:HD23	1:B:385[A]:VAL:HG13	1.53	0.91
1:B:92[A]:GLU:CD	1:B:384[A]:ASN:HD21	1.78	0.85
1:B:295:LEU:CD2	1:B:385[A]:VAL:HG13	2.10	0.81
1:A:374:LYS:HE2	1:A:384[B]:ASN:OD1	1.86	0.75
1:B:374:LYS:HE2	1:B:384[B]:ASN:OD1	1.87	0.75
1:B:92[A]:GLU:OE2	1:B:384[A]:ASN:ND2	2.22	0.73
1:B:83:LYS:HE2	10:B:1423:HOH:O	1.95	0.66
1:B:63:TYR:O	1:B:66:VAL:HG22	1.96	0.66
1:B:374:LYS:HD2	10:B:766:HOH:O	1.97	0.64
8:B:527:MAN:H4	10:B:1239:HOH:O	1.97	0.64
1:B:110:ASN:HB2	2:B:522:FAD:N5	2.15	0.61
1:A:374:LYS:CE	1:A:384[B]:ASN:HD21	2.14	0.61
1:A:110:ASN:HB2	2:A:522:FAD:N5	2.15	0.60
1:B:92[A]:GLU:CD	1:B:384[A]:ASN:ND2	2.52	0.60
8:B:527:MAN:H5	10:B:1336:HOH:O	2.01	0.60
1:A:132:ASP:O	1:A:136:GLN:HG3	2.02	0.59
1:B:237:ASP:OD2	1:B:243:HIS:HE1	1.84	0.59
1:A:150:ASN:ND2	1:A:190:ASN:ND2	2.43	0.59
1:B:511:ILE:O	1:B:515:GLN:HG3	2.03	0.59
1:B:374:LYS:HG2	1:B:384[B]:ASN:ND2	2.17	0.58
1:A:237:ASP:OD2	1:A:243:HIS:HE1	1.86	0.58
1:B:74:TYR:O	1:B:78[A]:GLN:HG2	2.04	0.57
1:B:110:ASN:HB2	2:B:522:FAD:C5X	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:ILE:O	1:A:515:GLN:HG3	2.05	0.57
1:B:423:LEU:HB3	1:B:424:PRO:HD2	1.86	0.57
1:A:110:ASN:HB2	2:A:522:FAD:C5X	2.35	0.55
1:A:374:LYS:HE2	1:A:384[B]:ASN:HD21	1.71	0.55
1:B:41:LEU:HD21	1:B:254:ILE:HG21	1.88	0.54
1:A:374:LYS:HE2	1:A:384[B]:ASN:ND2	2.22	0.54
1:A:384[B]:ASN:ND2	10:A:944:HOH:O	2.30	0.54
1:A:260:ILE:HD12	1:A:385[A]:VAL:HG21	1.90	0.54
1:A:416:LYS:HE2	10:A:957:HOH:O	2.07	0.54
1:A:235:TYR:CZ	1:A:243:HIS:HB2	2.43	0.53
1:A:374:LYS:HE2	1:A:384[B]:ASN:CG	2.30	0.52
1:B:306:LEU:HD23	1:B:355:PHE:HB3	1.91	0.52
1:A:219:LYS:HE2	10:A:1263:HOH:O	2.09	0.52
1:A:63:TYR:O	1:A:66:VAL:HG22	2.10	0.52
1:A:295:LEU:HD22	1:A:463:GLY:HA2	1.91	0.52
1:A:260:ILE:HD12	1:A:385[B]:VAL:HG11	1.91	0.52
1:B:24:GLU:HG3	1:B:246:PHE:HE1	1.75	0.51
1:B:369:GLY:HA3	1:B:386:LYS:O	2.10	0.51
1:A:361:LYS:HB2	1:A:457:TYR:CD1	2.46	0.51
5:A:528:NAG:O7	5:A:529:FUC:H61	2.10	0.51
1:B:374:LYS:CE	1:B:384[B]:ASN:OD1	2.57	0.51
1:A:369:GLY:HA3	1:A:386:LYS:O	2.11	0.51
1:A:350:LEU:HD12	1:A:350:LEU:N	2.26	0.51
1:B:351:PRO:HB3	1:B:432:LEU:HD22	1.93	0.50
1:A:79:GLU:HG2	10:A:1123:HOH:O	2.11	0.50
1:B:361:LYS:HB2	1:B:457:TYR:CD1	2.47	0.50
1:A:517:ARG:O	1:A:521:ASP:HB2	2.12	0.50
1:A:74:TYR:O	1:A:78[A]:GLN:HG2	2.12	0.50
1:A:150:ASN:HD21	1:A:190:ASN:HB3	1.76	0.49
1:A:168:HIS:HB3	1:A:169:PRO:HA	1.94	0.49
1:B:260:ILE:HD12	1:B:385[B]:VAL:HG11	1.95	0.48
1:A:154:TRP:CD1	1:A:331:SER:HB3	2.49	0.48
1:A:419:LYS:HE2	1:A:429:PHE:CE1	2.48	0.48
1:B:260:ILE:HD12	1:B:385[A]:VAL:HG21	1.96	0.48
1:A:262:THR:HB	1:A:263:PRO:HD3	1.95	0.47
1:A:374:LYS:HG3	10:A:937:HOH:O	2.15	0.47
1:A:361:LYS:HB2	1:A:457:TYR:CE1	2.49	0.47
1:B:154:TRP:CD1	1:B:331:SER:HB3	2.50	0.47
1:B:262:THR:HB	1:B:263:PRO:HD3	1.96	0.47
1:A:392:ASN:HA	5:A:527:NAG:H82	1.98	0.46
1:B:361:LYS:HB2	1:B:457:TYR:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:LYS:HG2	1:B:384[B]:ASN:HD21	1.80	0.46
1:A:473:ASP:HB2	1:A:475[B]:ARG:NH1	2.31	0.46
1:B:89:PHE:CZ	1:B:97:ASN:HB3	2.51	0.46
1:B:132:ASP:O	1:B:136:GLN:HG3	2.16	0.45
1:B:195:HIS:HA	1:B:199:GLU:OE1	2.16	0.45
1:A:89:PHE:CZ	1:A:97:ASN:HB3	2.51	0.45
1:B:438:LYS:NZ	1:B:438:LYS:HB2	2.31	0.45
1:A:374:LYS:CE	1:A:384[B]:ASN:ND2	2.79	0.45
1:B:249:SER:O	1:B:250:LYS:HB2	2.16	0.45
1:B:498:PRO:HB2	1:B:502:TYR:CE1	2.52	0.45
1:B:168:HIS:HB3	1:B:169:PRO:HA	1.98	0.45
1:B:118:ASN:O	1:B:121:ILE:HG12	2.17	0.44
1:B:416:LYS:HB2	1:B:417:PRO:HD3	1.99	0.44
1:A:156:SER:O	1:A:160:THR:HG23	2.18	0.44
1:B:150:ASN:ND2	1:B:190:ASN:OD1	2.51	0.44
1:B:288:HIS:HB3	1:B:291:VAL:HG23	1.99	0.43
1:A:41:LEU:HD21	1:A:254:ILE:HG21	2.01	0.43
1:A:413:ASP:HA	1:A:416:LYS:CD	2.48	0.43
1:A:498:PRO:HB2	1:A:502:TYR:CE1	2.54	0.43
1:A:300:ARG:HB2	1:A:457:TYR:CD1	2.54	0.43
1:B:150:ASN:HD21	1:B:190:ASN:HB3	1.84	0.43
1:B:419:LYS:HE2	1:B:429:PHE:CE1	2.54	0.43
8:B:523:NAG:O6	8:B:525:FUC:H3	2.18	0.43
1:A:249:SER:O	1:A:250:LYS:HB2	2.19	0.42
1:A:118:ASN:O	1:A:121:ILE:HG12	2.19	0.42
1:A:296:HIS:HB3	1:A:365:PRO:HD2	2.00	0.42
1:A:118:ASN:HB3	1:A:121:ILE:HG23	2.01	0.42
1:B:416:LYS:N	1:B:417:PRO:CD	2.82	0.42
1:A:416:LYS:HB2	1:A:417:PRO:HD3	2.02	0.42
1:A:195:HIS:HA	1:A:199:GLU:OE1	2.19	0.42
1:B:191:LYS:NZ	10:B:1376:HOH:O	2.48	0.42
1:A:295:LEU:HD22	1:A:463:GLY:CA	2.49	0.42
1:A:338:PRO:HA	1:A:339:PRO:HD3	1.82	0.42
1:A:27:TYR:O	1:A:247:VAL:HA	2.19	0.42
1:A:366:LEU:HD12	1:A:394:THR:HB	2.01	0.42
1:B:173:PHE:HB2	7:B:535:MXN:H2	2.02	0.42
1:A:149:PRO:O	7:A:532:MXN:H4	2.20	0.41
1:A:497:HIS:HB3	2:A:522:FAD:O2	2.20	0.41
1:B:324:ASP:HB3	1:B:398:HIS:CG	2.54	0.41
1:B:334:PRO:HB3	1:B:353:SER:N	2.36	0.41
1:B:410:LEU:HA	1:B:415:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:HIS:HB3	2:B:522:FAD:O2	2.20	0.41
1:B:235:TYR:CZ	1:B:243:HIS:HB2	2.56	0.41
1:B:281:ASN:ND2	10:B:960:HOH:O	2.54	0.41
1:B:371:LEU:C	1:B:371:LEU:HD23	2.40	0.41
1:B:156:SER:O	1:B:160:THR:HG23	2.21	0.41
1:A:347:SER:OG	1:A:347:SER:O	2.36	0.41
1:A:147:TYR:CD1	1:A:147:TYR:N	2.88	0.41
1:A:416:LYS:N	1:A:417:PRO:CD	2.84	0.41
1:B:1:LEU:HD21	1:B:175:LEU:HD11	2.03	0.41
1:B:162:PHE:HA	1:B:409[A]:LEU:HD21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	527/521 (101%)	512 (97%)	14 (3%)	1 (0%)	51	30
1	B	528/521 (101%)	512 (97%)	16 (3%)	0	100	100
All	All	1055/1042 (101%)	1024 (97%)	30 (3%)	1 (0%)	55	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	486	ASP

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	451/443 (102%)	443 (98%)	8 (2%)	64	45
1	B	452/443 (102%)	449 (99%)	3 (1%)	87	79
All	All	903/886 (102%)	892 (99%)	11 (1%)	78	62

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	SER
1	A	288	HIS
1	A	335	PHE
1	A	336	THR
1	A	345[A]	SER
1	A	345[B]	SER
1	A	430	ASN
1	A	498	PRO
1	B	288	HIS
1	B	430	ASN
1	B	498	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	ASN
1	A	207	ASN
1	A	243	HIS
1	A	281	ASN
1	A	430	ASN
1	B	65	ASN
1	B	150	ASN
1	B	190	ASN
1	B	243	HIS
1	B	281	ASN
1	B	430	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

15 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	$\# Z > 2$
4	NAG	A	524	1,4	14,14,15	0.64	0	15,19,21	0.88	1 (6%)
4	NAG	A	525	4	14,14,15	0.66	0	15,19,21	0.73	0
4	MAN	A	526	4	11,11,12	0.57	0	13,15,17	0.47	0
5	NAG	A	527	1,5	14,14,15	0.51	0	15,19,21	0.82	1 (6%)
5	NAG	A	528	5	14,14,15	0.49	0	15,19,21	0.71	0
5	FUC	A	529	5	9,10,11	0.45	0	13,14,16	0.40	0
8	NAG	B	523	8	14,14,15	0.50	0	15,19,21	0.64	0
8	NAG	B	524	1,8	14,14,15	0.50	0	15,19,21	0.78	1 (6%)
8	FUC	B	525	8	9,10,11	0.45	0	13,14,16	0.39	0
8	BMA	B	526	8	11,11,12	0.47	0	13,15,17	0.28	0
8	MAN	B	527	8	11,11,12	0.47	0	13,15,17	0.58	0
9	NAG	B	528	1,9	14,14,15	0.58	0	15,19,21	1.25	2 (13%)
9	NAG	B	529	9	14,14,15	0.55	0	15,19,21	0.65	0
9	BMA	B	530	9	11,11,12	0.46	0	13,15,17	0.46	0
9	MAN	B	531	9	11,11,12	0.49	0	13,15,17	0.55	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	524	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	525	4	-	0/6/23/26	0/1/1/1
4	MAN	A	526	4	-	0/2/19/22	0/1/1/1
5	NAG	A	527	1,5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	528	5	-	0/6/23/26	0/1/1/1
5	FUC	A	529	5	-	0/0/17/20	0/1/1/1
8	NAG	B	523	8	-	0/6/23/26	0/1/1/1
8	NAG	B	524	1,8	-	0/6/23/26	0/1/1/1
8	FUC	B	525	8	-	0/0/17/20	0/1/1/1
8	BMA	B	526	8	-	0/2/19/22	0/1/1/1
8	MAN	B	527	8	-	0/2/19/22	0/1/1/1
9	NAG	B	528	1,9	-	0/6/23/26	0/1/1/1
9	NAG	B	529	9	-	0/6/23/26	0/1/1/1
9	BMA	B	530	9	-	0/2/19/22	0/1/1/1
9	MAN	B	531	9	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	528	NAG	C4-C3-C2	-3.05	106.56	111.02
8	B	524	NAG	C2-N2-C7	-2.23	119.69	122.94
9	B	528	NAG	C2-N2-C7	-2.21	119.72	122.94
5	A	527	NAG	C2-N2-C7	-2.19	119.75	122.94
4	A	524	NAG	C2-N2-C7	-2.04	119.96	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	527	NAG	1	0
5	A	528	NAG	1	0
5	A	529	FUC	1	0
8	B	523	NAG	1	0
8	B	525	FUC	1	0
8	B	527	MAN	2	0

5.6 Ligand geometry ⓘ

10 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
2	FAD	A	522	-	51,58,58	2.17	21 (41%)	54,89,89	1.71	9 (16%)
3	NAG	A	523	1	14,14,15	0.46	0	15,19,21	0.64	0
6	HBX	A	530	-	8,8,8	1.83	4 (50%)	9,9,9	0.72	0
7	MXN	A	531	-	10,10,10	2.13	5 (50%)	11,12,12	0.57	0
7	MXN	A	532	-	10,10,10	1.84	3 (30%)	11,12,12	0.63	0
2	FAD	B	522	-	51,58,58	2.21	20 (39%)	54,89,89	1.72	8 (14%)
3	NAG	B	532	1	14,14,15	0.50	0	15,19,21	0.62	0
6	HBX	B	533	-	8,8,8	1.81	2 (25%)	9,9,9	0.71	0
7	MXN	B	534	-	10,10,10	2.53	5 (50%)	11,12,12	0.60	0
7	MXN	B	535	-	10,10,10	1.88	4 (40%)	11,12,12	0.60	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	522	-	-	0/28/50/50	0/6/6/6
3	NAG	A	523	1	-	0/6/23/26	0/1/1/1
6	HBX	A	530	-	-	0/2/2/2	0/1/1/1
7	MXN	A	531	-	-	0/4/6/6	0/1/1/1
7	MXN	A	532	-	-	0/4/6/6	0/1/1/1
2	FAD	B	522	-	-	0/28/50/50	0/6/6/6
3	NAG	B	532	1	-	0/6/23/26	0/1/1/1
6	HBX	B	533	-	-	0/2/2/2	0/1/1/1
7	MXN	B	534	-	-	0/4/6/6	0/1/1/1
7	MXN	B	535	-	-	0/4/6/6	0/1/1/1

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	522	FAD	PA-O2A	-3.56	1.37	1.55
2	A	522	FAD	PA-O2A	-3.50	1.37	1.55
2	B	522	FAD	C5B-C4B	-3.27	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	522	FAD	C5B-C4B	-3.26	1.41	1.51
2	A	522	FAD	P-O2P	-3.01	1.40	1.55
2	B	522	FAD	P-O2P	-2.96	1.40	1.55
2	A	522	FAD	C2-N1	-2.36	1.33	1.38
2	B	522	FAD	C2-N1	-2.27	1.33	1.38
2	B	522	FAD	C2B-C1B	-2.27	1.50	1.53
2	A	522	FAD	C2B-C1B	-2.16	1.50	1.53
7	A	532	MXN	C3-C2	2.00	1.42	1.38
7	B	535	MXN	C3-C2	2.01	1.42	1.38
6	A	530	HBX	C3-C2	2.02	1.42	1.38
6	A	530	HBX	C5-C6	2.04	1.42	1.38
7	B	534	MXN	C4-C3	2.04	1.43	1.38
6	B	533	HBX	C5-C6	2.04	1.42	1.38
7	B	534	MXN	C5-C6	2.04	1.42	1.38
6	A	530	HBX	C5-C4	2.06	1.43	1.38
2	A	522	FAD	C3B-C4B	2.07	1.58	1.53
7	B	535	MXN	C5-C6	2.07	1.42	1.38
6	A	530	HBX	C6-C1	2.07	1.43	1.39
7	A	531	MXN	C3-C2	2.10	1.42	1.38
6	B	533	HBX	C3-C2	2.10	1.42	1.38
7	A	531	MXN	C5-C6	2.10	1.42	1.38
2	A	522	FAD	C5X-N5	2.16	1.38	1.35
2	B	522	FAD	C4A-N3A	2.24	1.38	1.35
7	A	531	MXN	C2-C1	2.25	1.42	1.39
2	A	522	FAD	C2A-N1A	2.26	1.38	1.33
2	B	522	FAD	C5X-N5	2.27	1.38	1.35
2	A	522	FAD	C4A-N3A	2.34	1.39	1.35
2	B	522	FAD	C2A-N1A	2.37	1.38	1.33
7	B	534	MXN	C2-C1	2.43	1.43	1.39
2	B	522	FAD	C2A-N3A	2.49	1.36	1.32
2	A	522	FAD	O4B-C4B	2.50	1.50	1.45
7	A	532	MXN	C2-C1	2.55	1.43	1.39
2	A	522	FAD	C2A-N3A	2.55	1.36	1.32
7	B	535	MXN	C2-C1	2.56	1.43	1.39
2	A	522	FAD	C4-C4X	2.58	1.46	1.41
2	B	522	FAD	O4B-C4B	2.58	1.50	1.45
2	A	522	FAD	C2-N3	2.81	1.43	1.38
7	A	532	MXN	C6-C1	2.83	1.43	1.39
2	A	522	FAD	O5'-C5'	2.84	1.56	1.44
2	B	522	FAD	C2-N3	2.84	1.43	1.38
2	B	522	FAD	O5'-C5'	2.86	1.56	1.44
7	B	535	MXN	C6-C1	2.86	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	522	FAD	C8-C7	2.88	1.48	1.41
2	B	522	FAD	C4-C4X	2.93	1.46	1.41
2	A	522	FAD	C8-C7	2.94	1.48	1.41
2	A	522	FAD	C10-N1	3.06	1.37	1.33
7	B	534	MXN	C6-C1	3.08	1.44	1.39
7	A	531	MXN	C7-C8	3.09	1.57	1.48
2	A	522	FAD	C4X-N5	3.12	1.37	1.33
7	A	531	MXN	C6-C1	3.15	1.44	1.39
2	B	522	FAD	C4X-N5	3.25	1.38	1.33
2	B	522	FAD	C10-N1	3.64	1.38	1.33
2	A	522	FAD	C4-N3	3.81	1.39	1.33
2	B	522	FAD	C4-N3	3.89	1.40	1.33
2	B	522	FAD	O4B-C1B	4.14	1.47	1.41
2	A	522	FAD	C4X-C10	4.26	1.48	1.41
2	B	522	FAD	C4X-C10	4.32	1.48	1.41
2	A	522	FAD	O4B-C1B	4.44	1.47	1.41
7	B	534	MXN	C7-C8	5.35	1.64	1.48
2	A	522	FAD	C9A-N10	5.99	1.46	1.38
2	B	522	FAD	C9A-N10	6.27	1.47	1.38

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	522	FAD	C4X-C4-N3	-4.39	117.23	123.48
2	A	522	FAD	C4X-C4-N3	-4.39	117.24	123.48
2	A	522	FAD	N3A-C2A-N1A	-3.39	125.91	128.86
2	B	522	FAD	N3A-C2A-N1A	-3.19	126.08	128.86
2	B	522	FAD	C4-C4X-C10	-3.07	117.48	119.96
2	A	522	FAD	C4-C4X-C10	-2.94	117.58	119.96
2	B	522	FAD	O5B-PA-O1A	-2.61	98.70	109.25
2	A	522	FAD	O5B-PA-O1A	-2.51	99.10	109.25
2	B	522	FAD	C4X-C10-N10	-2.48	118.80	120.52
2	A	522	FAD	C4X-C10-N10	-2.32	118.91	120.52
2	A	522	FAD	C5X-C9A-N10	-2.17	116.04	117.66
2	B	522	FAD	C5X-C9A-N10	-2.15	116.06	117.66
2	A	522	FAD	C4A-C5A-N7A	2.03	111.37	109.41
2	B	522	FAD	C2A-N1A-C6A	2.20	122.62	118.77
2	A	522	FAD	C2A-N1A-C6A	2.27	122.75	118.77
2	A	522	FAD	C4-N3-C2	7.58	121.79	115.16
2	B	522	FAD	C4-N3-C2	7.77	121.96	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	522	FAD	3	0
7	A	532	MXN	1	0
2	B	522	FAD	3	0
7	B	535	MXN	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	521/521 (100%)	-0.40	8 (1%) 74 78	7, 12, 24, 48	0
1	B	521/521 (100%)	-0.36	6 (1%) 79 83	7, 13, 26, 42	0
All	All	1042/1042 (100%)	-0.38	14 (1%) 77 81	7, 13, 26, 48	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	225	ALA	4.2
1	A	336	THR	3.9
1	A	521	ASP	3.8
1	A	422	ASP	3.0
1	A	520	SER	3.0
1	B	422	ASP	2.9
1	B	519	ALA	2.8
1	A	519	ALA	2.6
1	A	124	ALA	2.5
1	B	124	ALA	2.5
1	B	521	ASP	2.5
1	B	23	LEU	2.3
1	B	424	PRO	2.1
1	A	335	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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
5	NAG	A	527	14/15	0.81	0.16	12.07	27,33,40,41	0
9	NAG	B	528	14/15	0.82	0.12	3.33	16,21,25,25	0
8	MAN	B	527	11/12	0.63	0.25	1.38	48,50,50,50	0
4	NAG	A	524	14/15	0.90	0.10	1.36	13,19,22,23	0
8	NAG	B	524	14/15	0.88	0.14	-	21,26,29,30	0
4	MAN	A	526	11/12	0.58	0.28	-	46,49,50,51	0
8	FUC	B	525	10/11	0.88	0.29	-	33,35,36,37	0
8	BMA	B	526	11/12	0.66	0.29	-	42,44,46,47	0
9	BMA	B	530	11/12	0.62	0.30	-	45,47,50,53	0
8	NAG	B	523	14/15	0.88	0.22	-	31,32,38,38	0
9	MAN	B	531	11/12	0.36	0.42	-	54,55,56,56	0
5	NAG	A	528	14/15	0.78	0.34	-	45,48,49,49	0
4	NAG	A	525	14/15	0.75	0.19	-	27,30,38,42	0
9	NAG	B	529	14/15	0.76	0.20	-	30,32,40,41	0
5	FUC	A	529	10/11	0.74	0.33	-	44,46,47,47	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
7	MXN	B	535	10/10	0.85	0.24	8.74	40,41,42,43	0
7	MXN	A	532	10/10	0.75	0.21	4.96	36,38,38,40	0
7	MXN	A	531	10/10	0.91	0.10	3.86	14,15,17,23	0
7	MXN	B	534	10/10	0.91	0.10	3.60	14,17,18,23	0
6	HBX	B	533	8/8	0.95	0.08	1.30	20,23,23,23	0
6	HBX	A	530	8/8	0.95	0.08	1.19	21,21,22,22	0
3	NAG	A	523	14/15	0.93	0.08	0.09	14,17,20,21	0
2	FAD	A	522	53/53	0.98	0.06	-0.41	5,8,9,10	0
3	NAG	B	532	14/15	0.94	0.07	-0.47	14,16,21,21	0
2	FAD	B	522	53/53	0.98	0.06	-0.59	6,8,10,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.