



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 01:16 AM 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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

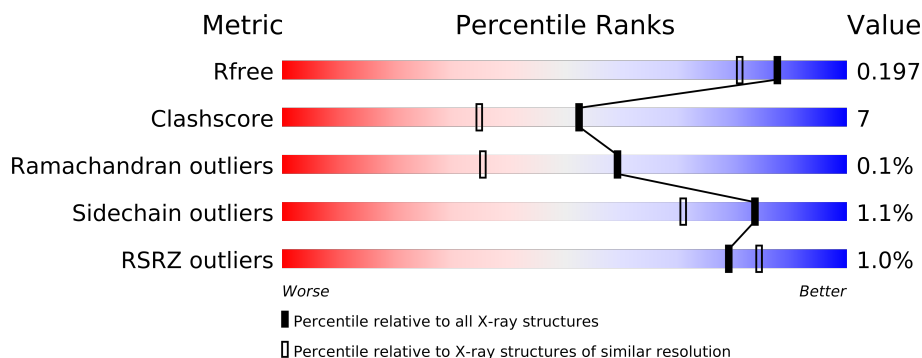
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance



The reported resolution of this entry is 1.67 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}	66092	3587 (1.70-1.66)
Clashscore	79885	4225 (1.70-1.66)
Ramachandran outliers	78287	4144 (1.70-1.66)
Sidechain outliers	78261	4143 (1.70-1.66)
RSRZ outliers	66119	3587 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	521	
1	B	521	

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

Mol	Type	Chain	Res	Geometry	Electron density
6	HBX	B	533	-	X
7	MXN	A	531	-	X
7	MXN	A	532	-	X
7	MXN	B	534	-	X
7	MXN	B	535	-	X

2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 9681 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

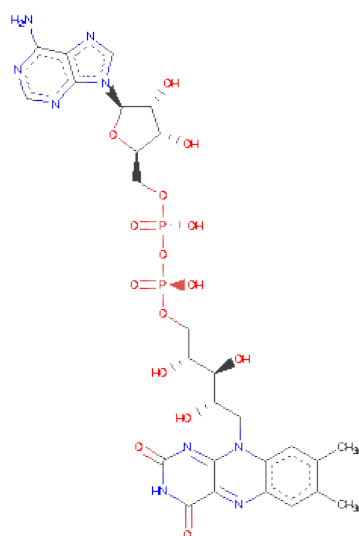
- Molecule 1 is a protein called R-oxynitrile lyase isoenzyme 1.

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



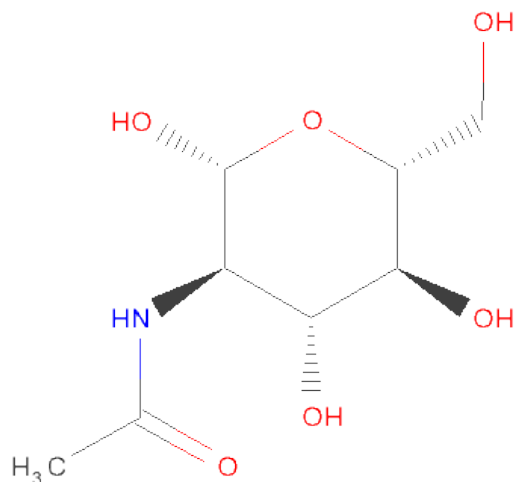
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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

- 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		

There is a discrepancy between the modelled and reference sequences:

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

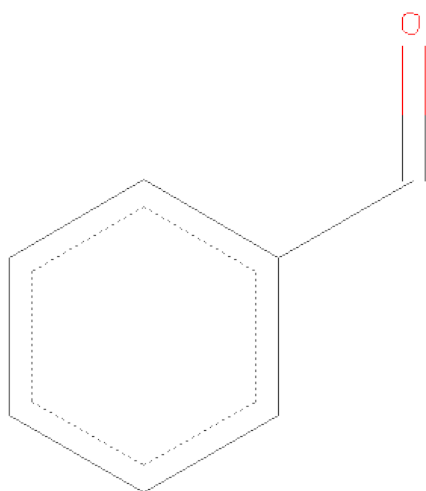
- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

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

There is a discrepancy between the modelled and reference sequences:

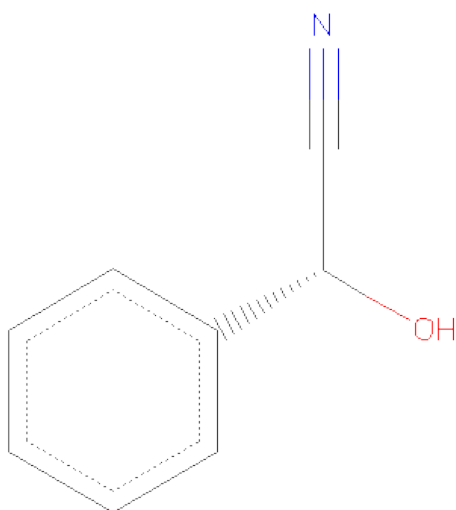
Chain	Residue	Modelled	Actual	Comment	Reference
A	346	SER	ALA	SEE REMARK 999	UNP Q945K2

- Molecule 6 is BENZALDEHYDE (three-letter code: HBX) (formula: C₇H₆O).



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		
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		

There is a discrepancy between the modelled and reference sequences:

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

- 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		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 10 is water.

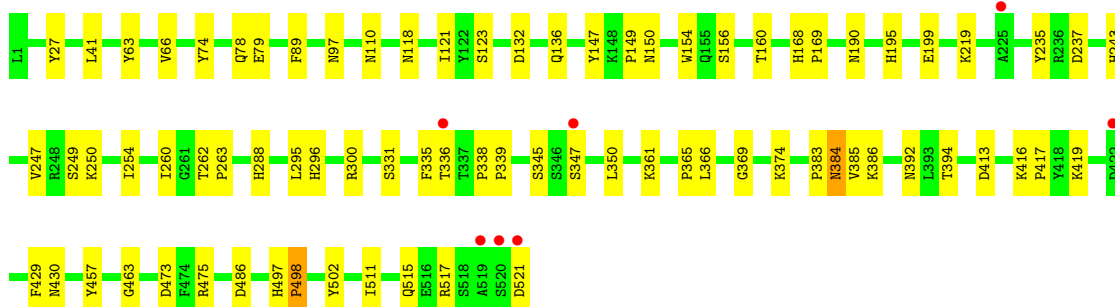
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	643	Total O 643 643	0	0
10	B	626	Total O 626 626	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

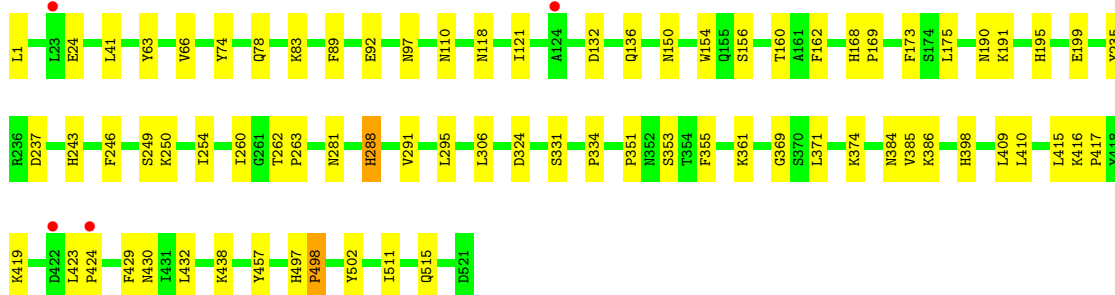
- Molecule 1: R-oxynitrile lyase isoenzyme 1

Chain A: 



- Molecule 1: R-oxynitrile lyase isoenzyme 1

Chain B: 



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 0.176 , 0.197	Depositor DCC
R_{free} test set	10601 reflections (11.09%)	DCC
Wilson B-factor (Å ²)	13.5	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	3 of 107934 reflections (0.003%)	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.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	14	0	13	0	0
4	A	39	0	34	0	0
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

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

All (117) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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:416:LYS:HE2	10:A:957:HOH:O	2.07	0.54
1:A:260:ILE:HD12	1:A:385[A]:VAL:HG21	1.90	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:260:ILE:HD12	1:A:385[B]:VAL:HG11	1.91	0.52
1:A:295:LEU:HD22	1:A:463:GLY:HA2	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
5:A:528:NAG:O7	5:A:529:FUC:H61	2.10	0.51
1:A:361:LYS:HB2	1:A:457:TYR:CD1	2.46	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:419:LYS:HE2	1:A:429:PHE:CE1	2.48	0.48
1:A:154:TRP:CD1	1:A:331:SER:HB3	2.49	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:374:LYS:HG2	1:B:384[B]:ASN:HD21	1.80	0.46
1:B:361:LYS:HB2	1:B:457:TYR:CE1	2.50	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:416:LYS:N	1:B:417:PRO:CD	2.82	0.42
1:A:118:ASN:HB3	1:A:121:ILE:HG23	2.01	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:497:HIS:HB3	2:B:522:FAD:O2	2.20	0.41
1:B:410:LEU:HA	1:B:415:LEU:HD12	2.01	0.41
1:B:235:TYR:CZ	1:B:243:HIS:HB2	2.56	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:A:147:TYR:N	1:A:147:TYR:CD1	2.88	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

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	527/521 (101%)	512 (97%)	14 (3%)	1 (0%)	56	32
1	B	528/521 (101%)	512 (97%)	16 (3%)	0	100	100
All	All	1055/1042 (101%)	1024 (97%)	30 (3%)	1 (0%)	59	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	486	ASP

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	451/443 (102%)	443 (98%)	8 (2%)	71	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	452/443 (102%)	449 (99%)	3 (1%)	91	84
All	All	903/886 (102%)	892 (99%)	11 (1%)	84	67

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 chains in this entry.

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

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

5.5 Carbohydrates ⓘ

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	12,14,15	0.52	0	15,19,21	0.90	0
4	NAG	A	525	4	12,14,15	0.60	0	15,19,21	0.85	0
4	MAN	A	526	4	10,11,12	0.42	0	11,15,17	0.35	0
5	NAG	A	527	1,5	12,14,15	0.50	0	15,19,21	0.72	0
5	NAG	A	528	5	12,14,15	0.41	0	15,19,21	0.70	0
5	FUC	A	529	5	9,10,11	0.41	0	10,14,16	0.27	0
8	NAG	B	523	8	12,14,15	0.48	0	15,19,21	0.72	0
8	NAG	B	524	1,8	12,14,15	0.50	0	15,19,21	0.71	1 (6%)
8	FUC	B	525	8	9,10,11	0.41	0	10,14,16	0.26	0
8	BMA	B	526	8	10,11,12	0.42	0	11,15,17	0.28	0
8	MAN	B	527	8	10,11,12	0.40	0	11,15,17	0.23	0
9	NAG	B	528	1,9	12,14,15	0.50	0	15,19,21	1.12	1 (6%)
9	NAG	B	529	9	12,14,15	0.54	0	15,19,21	0.70	0
9	BMA	B	530	9	10,11,12	0.42	0	11,15,17	0.41	0
9	MAN	B	531	9	10,11,12	0.39	0	11,15,17	0.21	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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	524	NAG	C2-N2-C7	-2.02	119.69	123.09
9	B	528	NAG	C2-N2-C7	-2.00	119.72	123.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	-	58,58,58	2.15	19 (32%)	85,89,89	1.50	10 (11%)
3	NAG	A	523	1	12,14,15	0.46	0	15,19,21	0.68	0
6	HBX	A	530	-	8,8,8	1.67	1 (12%)	9,9,9	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MXN	A	531	-	10,10,10	2.06	4 (40%)	12,12,12	0.59	0
7	MXN	A	532	-	10,10,10	1.71	2 (20%)	12,12,12	0.67	0
2	FAD	B	522	-	58,58,58	2.20	20 (34%)	85,89,89	1.48	10 (11%)
3	NAG	B	532	1	12,14,15	0.50	0	15,19,21	0.67	0
6	HBX	B	533	-	8,8,8	1.64	0	9,9,9	0.71	0
7	MXN	B	534	-	10,10,10	2.54	4 (40%)	12,12,12	0.63	0
7	MXN	B	535	-	10,10,10	1.75	3 (30%)	12,12,12	0.64	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	-	-	0/34/50/50	0/1/6/6
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	-	-	0/34/50/50	0/1/6/6
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 (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	522	FAD	P-O3P	-6.80	1.47	1.59
2	A	522	FAD	P-O3P	-6.67	1.47	1.59
7	B	534	MXN	C7-C8	5.80	1.64	1.48
2	B	522	FAD	C9A-N10	5.49	1.47	1.38
2	A	522	FAD	C9A-N10	5.24	1.46	1.38
2	B	522	FAD	C4X-C10	4.43	1.48	1.40
2	A	522	FAD	C4X-C10	4.36	1.48	1.40
2	B	522	FAD	PA-O2A	-3.99	1.37	1.55
2	A	522	FAD	O4B-C1B	3.94	1.47	1.41
2	A	522	FAD	PA-O2A	-3.92	1.37	1.55
2	B	522	FAD	O4B-C1B	3.67	1.47	1.41
2	B	522	FAD	C4-C4X	3.50	1.46	1.41
7	A	531	MXN	C7-C8	3.40	1.57	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	522	FAD	P-O2P	-3.37	1.40	1.55
2	B	522	FAD	C2-N3	3.33	1.43	1.37
2	B	522	FAD	P-O2P	-3.32	1.40	1.55
2	A	522	FAD	C2-N3	3.29	1.43	1.37
2	A	522	FAD	C1'-C2'	3.27	1.54	1.51
2	B	522	FAD	C5B-C4B	-3.19	1.41	1.51
2	A	522	FAD	C5B-C4B	-3.18	1.41	1.51
2	B	522	FAD	C1'-C2'	3.15	1.54	1.51
2	A	522	FAD	C4-C4X	3.09	1.46	1.41
7	A	531	MXN	C6-C1	3.00	1.44	1.39
7	B	534	MXN	C6-C1	2.93	1.44	1.39
2	B	522	FAD	O5'-C5'	2.74	1.56	1.44
2	B	522	FAD	PA-O3P	2.73	1.64	1.59
7	B	535	MXN	C6-C1	2.73	1.43	1.39
2	A	522	FAD	O5'-C5'	2.71	1.56	1.44
7	A	532	MXN	C6-C1	2.70	1.43	1.39
2	A	522	FAD	C8-C7	2.61	1.48	1.40
2	B	522	FAD	C8-C7	2.56	1.48	1.40
2	B	522	FAD	O4B-C4B	2.49	1.50	1.45
7	B	535	MXN	C2-C1	2.44	1.43	1.39
7	A	532	MXN	C2-C1	2.43	1.43	1.39
2	A	522	FAD	O4B-C4B	2.41	1.50	1.45
2	B	522	FAD	C2B-C1B	-2.40	1.50	1.53
7	B	534	MXN	C2-C1	2.33	1.43	1.39
2	A	522	FAD	C2B-C1B	-2.28	1.50	1.53
2	B	522	FAD	C5X-N5	2.28	1.38	1.35
2	B	522	FAD	C2A-N1A	2.26	1.38	1.33
2	A	522	FAD	PA-O3P	2.23	1.63	1.59
2	A	522	FAD	C4A-N3A	2.22	1.39	1.35
2	A	522	FAD	C5X-N5	2.17	1.38	1.35
2	A	522	FAD	C2A-N3A	2.15	1.36	1.32
7	A	531	MXN	C2-C1	2.15	1.42	1.39
2	A	522	FAD	C2A-N1A	2.15	1.38	1.33
2	B	522	FAD	C4A-N3A	2.13	1.38	1.35
2	B	522	FAD	C2A-N3A	2.10	1.36	1.32
6	A	530	HBX	C6-C1	2.09	1.43	1.39
2	B	522	FAD	C6-C5X	2.09	1.44	1.41
7	B	534	MXN	C1-C7	2.04	1.54	1.51
7	B	535	MXN	C1-C7	2.01	1.54	1.51
7	A	531	MXN	C1-C7	2.01	1.54	1.51

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	522	FAD	O4B-C1B-N9A	-6.98	101.95	108.44
2	B	522	FAD	O4B-C1B-N9A	-6.70	102.21	108.44
2	A	522	FAD	C2-N1-C10	5.91	120.93	114.98
2	B	522	FAD	C2-N1-C10	5.89	120.92	114.98
2	B	522	FAD	C4X-C10-N10	-3.43	118.80	120.51
2	A	522	FAD	N3A-C2A-N1A	-3.35	125.91	128.71
2	A	522	FAD	C4X-C10-N10	-3.20	118.91	120.51
2	B	522	FAD	N3A-C2A-N1A	-3.15	126.08	128.71
2	B	522	FAD	O5B-PA-O1A	-2.72	98.70	109.37
2	A	522	FAD	O5B-PA-O1A	-2.62	99.10	109.37
2	B	522	FAD	C5'-C4'-C3'	-2.34	107.64	112.06
2	A	522	FAD	C5'-C4'-C3'	-2.34	107.64	112.06
2	B	522	FAD	N3A-C4A-N9A	2.32	129.62	125.43
2	A	522	FAD	N3A-C4A-N9A	2.28	129.56	125.43
2	A	522	FAD	C5A-C4A-N9A	-2.26	103.90	107.16
2	B	522	FAD	C5A-C4A-N9A	-2.24	103.92	107.16
2	A	522	FAD	C2A-N1A-C6A	2.20	122.75	118.77
2	A	522	FAD	C4A-C5A-N7A	2.16	111.37	109.52
2	B	522	FAD	C2A-N1A-C6A	2.13	122.62	118.77
2	B	522	FAD	C4A-C5A-N7A	2.10	111.32	109.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	521/521 (100%)	-0.49	7 (1%) 74 79	7, 12, 24, 48	0
1	B	521/521 (100%)	-0.44	4 (0%) 83 88	7, 13, 26, 42	0
All	All	1042/1042 (100%)	-0.46	11 (1%) 79 83	7, 13, 26, 48	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	336	THR	3.3
1	A	225	ALA	3.2
1	A	521	ASP	3.0
1	A	422	ASP	2.8
1	A	520	SER	2.5
1	B	124	ALA	2.2
1	A	519	ALA	2.2
1	B	422	ASP	2.1
1	B	23	LEU	2.1
1	B	424	PRO	2.1
1	A	347	SER	2.0

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

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	MAN	B	531	11/12	0.37	63.07	54,55,56,56	0
9	NAG	B	529	14/15	0.20	41.09	30,32,40,41	0
4	NAG	A	525	14/15	0.19	17.07	27,30,38,42	0
5	NAG	A	527	14/15	0.15	12.07	27,33,40,41	0
8	NAG	B	524	14/15	0.13	8.33	21,26,29,30	0
9	NAG	B	528	14/15	0.12	4.96	16,21,25,25	0
4	NAG	A	524	14/15	0.09	1.25	13,19,22,23	0
8	MAN	B	527	11/12	0.21	1.08	48,50,50,50	0
9	BMA	B	530	11/12	0.27	-	45,47,50,53	0
8	NAG	B	523	14/15	0.18	-	31,32,38,38	0
4	MAN	A	526	11/12	0.27	-	46,49,50,51	0
5	NAG	A	528	14/15	0.31	-	45,48,49,49	0
8	FUC	B	525	10/11	0.25	-	33,35,36,37	0
8	BMA	B	526	11/12	0.24	-	42,44,46,47	0
5	FUC	A	529	10/11	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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	MXN	B	535	10/10	0.24	7.20	40,41,42,43	0
7	MXN	A	531	10/10	0.10	4.98	14,15,17,23	0
7	MXN	A	532	10/10	0.19	4.76	36,38,38,40	0
7	MXN	B	534	10/10	0.09	3.84	14,17,18,23	0
6	HBX	B	533	8/8	0.08	2.45	20,23,23,23	0
6	HBX	A	530	8/8	0.07	0.86	21,21,22,22	0
3	NAG	A	523	14/15	0.07	0.13	14,17,20,21	0
3	NAG	B	532	14/15	0.07	-0.21	14,16,21,21	0
2	FAD	A	522	53/53	0.05	-0.23	5,8,9,10	0
2	FAD	B	522	53/53	0.05	-0.32	6,8,10,11	0

6.5 Other polymers ⓘ

There are no such residues in this entry.