



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 07:39 PM EDT

PDB ID : 3OAH  
Title : Structural Characterization of the Dual Glycan Binding Adeno-Associated Virus Serotype 6  
Authors : Ng, R.; Agbandje-McKenna, M.  
Deposited on : 2010-08-05  
Resolution : 3.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

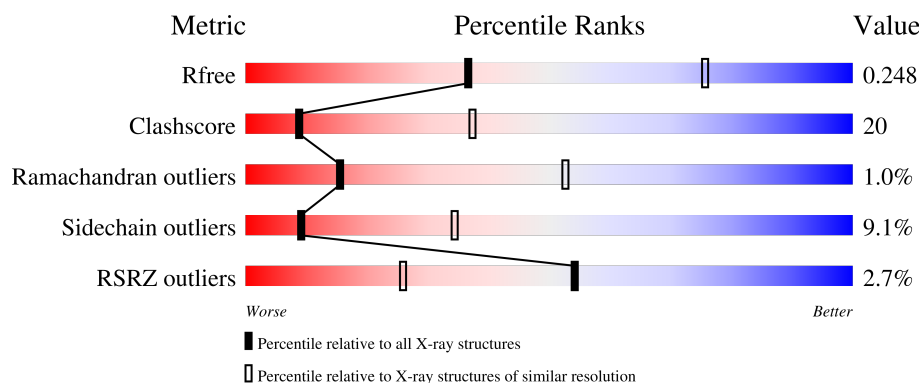
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


The reported resolution of this entry is 3.00 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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	534	

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
3	OAH	A	999	-	-	-	X

## 2 Entry composition [i](#)

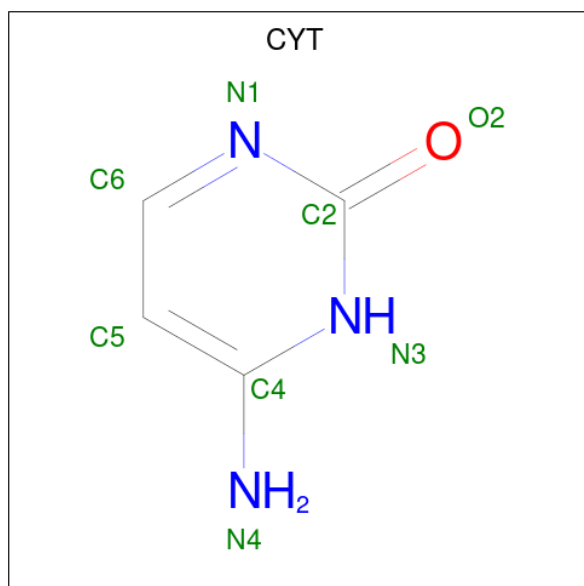
There are 4 unique types of molecules in this entry. The entry contains 4158 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Capsid protein VP1.

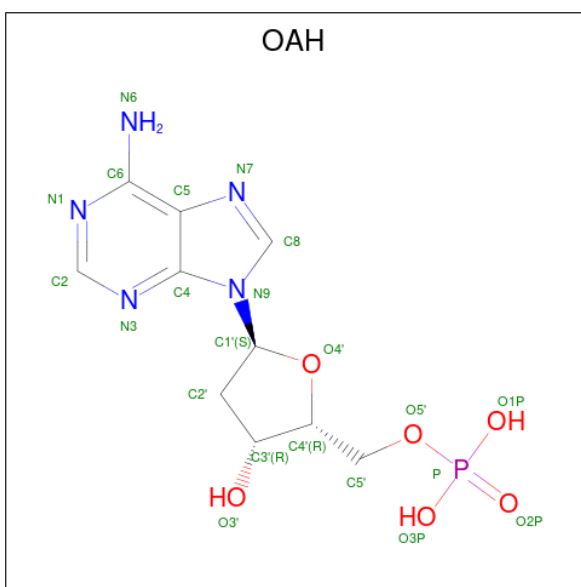
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	519	4117	2605	711	785	16	1	0	0

- Molecule 2 is 6-AMINOPYRIMIDIN-2(1H)-ONE (three-letter code: CYT) (formula:  $C_4H_5N_3O$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	8	4	3	1	0	0

- Molecule 3 is 9-(2-deoxy-5-O-phosphono-alpha-D-threo-pentofuranosyl)-9H-purin-6-amine (three-letter code: OAH) (formula:  $C_{10}H_{14}N_5O_6P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

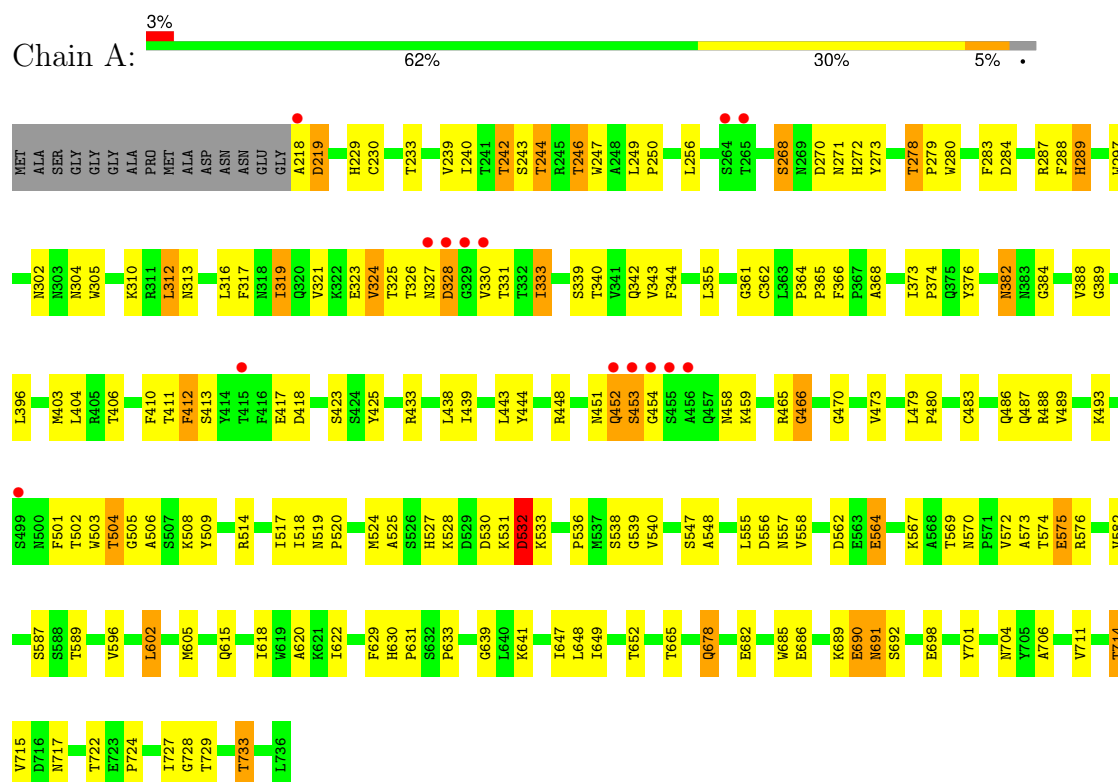
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	11	Total	O	0	0
			11	11		

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Capsid protein VP1



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	263.00Å 263.00Å 609.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.00 39.66 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.00) 63.5 (39.66-3.00)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.92 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.275 , 0.287 0.246 , 0.248	Depositor DCC
$R_{free}$ test set	5598 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.1	Xtriage
Anisotropy	1.092	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 35.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	4158	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CYT, OAH

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	0.46	0/4243	0.69	0/5785

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4117	0	3893	164	0
2	A	8	0	4	0	0
3	A	22	0	12	4	0
4	A	11	0	0	0	0
All	All	4158	0	3909	164	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 20.

All (164) 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:278:THR:HG23	1:A:280:TRP:H	1.11	1.16
1:A:218:ALA:CB	1:A:219:ASP:HA	1.76	1.10
1:A:218:ALA:HB1	1:A:219:ASP:HA	1.03	1.03
1:A:218:ALA:HB1	1:A:219:ASP:CA	1.91	0.99
1:A:622:ILE:HD12	1:A:631:PRO:HB2	1.51	0.93
1:A:333:ILE:HD12	1:A:333:ILE:H	1.42	0.83
1:A:278:THR:HG23	1:A:280:TRP:N	1.96	0.79
1:A:569:THR:HG23	1:A:570:ASN:OD1	1.85	0.76
1:A:302:ASN:HD21	1:A:701:TYR:H	1.34	0.76
1:A:361:GLY:HA3	1:A:374:PRO:HG3	1.66	0.75
1:A:451:ASN:ND2	1:A:458:ASN:HB2	2.02	0.75
1:A:531:LYS:C	1:A:533:LYS:H	1.90	0.74
1:A:229:HIS:O	1:A:244:THR:HG22	1.89	0.73
1:A:230:CYS:HB2	1:A:244:THR:HG22	1.73	0.71
1:A:698:GLU:OE1	1:A:733:THR:HB	1.91	0.70
1:A:722:THR:O	1:A:724:PRO:HD3	1.92	0.70
1:A:247:TRP:HB2	1:A:373:ILE:HD11	1.74	0.69
1:A:487:GLN:HE21	1:A:488:ARG:H	1.41	0.69
1:A:249:LEU:HD12	1:A:250:PRO:HD2	1.75	0.69
1:A:641:LYS:HE2	3:A:999:OAH:O1P	1.91	0.69
1:A:382:ASN:HD21	1:A:514:ARG:HH12	1.43	0.66
1:A:548:ALA:HB2	1:A:557:ASN:O	1.96	0.66
1:A:342:GLN:OE1	1:A:652:THR:HG22	1.96	0.66
1:A:480:PRO:O	1:A:605:MET:HG2	1.96	0.66
1:A:639:GLY:O	3:A:999:OAH:H2'	1.96	0.65
1:A:247:TRP:HB2	1:A:373:ILE:CD1	2.28	0.64
1:A:289:HIS:CE1	1:A:365:PRO:HG3	2.32	0.63
1:A:508:LYS:HG2	1:A:517:ILE:HD12	1.81	0.62
1:A:517:ILE:HG22	1:A:519:ASN:HB2	1.81	0.62
1:A:524:MET:HB2	1:A:573:ALA:HB2	1.82	0.61
1:A:284:ASP:OD1	1:A:355:LEU:HD22	2.01	0.61
1:A:527:HIS:HE2	1:A:532:ASP:CG	2.04	0.61
1:A:324:VAL:HG23	1:A:331:THR:HG22	1.80	0.61
1:A:403:MET:C	1:A:404:LEU:HD12	2.21	0.60
1:A:639:GLY:O	3:A:999:OAH:H8	2.01	0.60
1:A:487:GLN:NE2	1:A:488:ARG:H	1.98	0.59
1:A:704:ASN:HD21	1:A:706:ALA:HB3	1.67	0.59
1:A:691:ASN:HD22	1:A:691:ASN:C	2.05	0.59
1:A:711:VAL:O	1:A:714:THR:HB	2.03	0.59
1:A:555:LEU:HD23	1:A:555:LEU:C	2.23	0.59
1:A:555:LEU:HD23	1:A:555:LEU:O	2.03	0.59
1:A:629:PHE:O	1:A:630:HIS:C	2.41	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:LEU:HB2	1:A:605:MET:CE	2.33	0.59
1:A:326:THR:HB	1:A:331:THR:HG23	1.85	0.58
1:A:622:ILE:CD1	1:A:631:PRO:HB2	2.31	0.58
1:A:564:GLU:O	1:A:567:LYS:HG2	2.04	0.58
1:A:239:VAL:HG13	1:A:685:TRP:HB2	1.86	0.58
1:A:297:TRP:HE1	1:A:727:ILE:HG22	1.69	0.58
1:A:312:LEU:C	1:A:312:LEU:HD12	2.24	0.57
1:A:527:HIS:NE2	1:A:532:ASP:OD2	2.38	0.57
1:A:278:THR:CG2	1:A:280:TRP:H	2.01	0.56
1:A:504:THR:HG22	1:A:505:GLY:N	2.19	0.56
1:A:246:THR:HB	1:A:678:GLN:NE2	2.19	0.56
1:A:459:LYS:NZ	1:A:587:SER:HB3	2.21	0.56
1:A:691:ASN:C	1:A:691:ASN:ND2	2.59	0.56
1:A:501:PHE:HA	1:A:504:THR:HB	1.87	0.55
1:A:451:ASN:HD22	1:A:458:ASN:HB2	1.72	0.55
1:A:704:ASN:ND2	1:A:706:ALA:HB3	2.21	0.55
1:A:288:PHE:N	1:A:618:ILE:HD11	2.22	0.54
1:A:388:VAL:HG12	1:A:389:GLY:N	2.22	0.54
1:A:417:GLU:OE1	1:A:641:LYS:N	2.39	0.54
1:A:327:ASN:HB3	1:A:328:ASP:OD1	2.07	0.53
1:A:412:PHE:CE2	1:A:647:ILE:HD11	2.43	0.53
1:A:304:ASN:OD1	1:A:689:LYS:HD3	2.07	0.53
1:A:531:LYS:C	1:A:533:LYS:N	2.61	0.53
1:A:239:VAL:HG13	1:A:239:VAL:O	2.08	0.53
1:A:343:VAL:O	1:A:344:PHE:HB3	2.09	0.52
1:A:229:HIS:O	1:A:244:THR:CG2	2.57	0.52
1:A:602:LEU:HB2	1:A:605:MET:HE2	1.92	0.52
1:A:388:VAL:HG12	1:A:389:GLY:H	1.73	0.52
1:A:411:THR:HG22	1:A:412:PHE:N	2.24	0.52
1:A:488:ARG:HB2	1:A:574:THR:HB	1.92	0.52
1:A:396:LEU:HD13	1:A:648:LEU:HD13	1.92	0.52
1:A:622:ILE:HD11	1:A:639:GLY:HA3	1.92	0.52
1:A:284:ASP:O	1:A:362:CYS:HA	2.10	0.51
1:A:230:CYS:HB2	1:A:244:THR:CG2	2.40	0.51
1:A:230:CYS:HA	1:A:242:THR:O	2.10	0.51
1:A:582:VAL:HG12	1:A:582:VAL:O	2.11	0.51
1:A:242:THR:HB	1:A:682:GLU:HG3	1.93	0.51
1:A:278:THR:HG22	1:A:376:TYR:O	2.11	0.51
1:A:280:TRP:NE1	1:A:396:LEU:HB2	2.27	0.50
1:A:310:LYS:HD2	1:A:686:GLU:OE1	2.11	0.49
1:A:239:VAL:CG1	1:A:685:TRP:HB2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ILE:C	1:A:319:ILE:HD12	2.32	0.49
1:A:641:LYS:CE	3:A:999:OAH:O1P	2.60	0.49
1:A:326:THR:CB	1:A:331:THR:HG23	2.42	0.49
1:A:536:PRO:HD2	1:A:540:VAL:HG13	1.95	0.49
1:A:459:LYS:HZ3	1:A:587:SER:HB3	1.76	0.49
1:A:620:ALA:HB3	1:A:633:PRO:HG3	1.95	0.48
1:A:470:GLY:O	1:A:473:VAL:HG12	2.12	0.48
1:A:527:HIS:NE2	1:A:532:ASP:CG	2.66	0.48
1:A:412:PHE:HE2	1:A:647:ILE:HD11	1.77	0.48
1:A:382:ASN:HD21	1:A:514:ARG:NH1	2.10	0.48
1:A:527:HIS:CD2	1:A:532:ASP:HA	2.49	0.48
1:A:328:ASP:C	1:A:330:VAL:H	2.16	0.47
1:A:240:ILE:N	1:A:240:ILE:HD12	2.30	0.47
1:A:343:VAL:HG12	1:A:344:PHE:N	2.30	0.47
1:A:602:LEU:HB2	1:A:605:MET:HE3	1.97	0.47
1:A:342:GLN:HG2	1:A:403:MET:HG2	1.96	0.47
1:A:268:SER:HB3	1:A:271:ASN:HD22	1.79	0.47
1:A:273:TYR:C	1:A:273:TYR:CD1	2.88	0.47
1:A:324:VAL:HG23	1:A:331:THR:CG2	2.45	0.47
1:A:502:THR:O	1:A:506:ALA:HB2	2.14	0.47
1:A:531:LYS:O	1:A:533:LYS:N	2.48	0.46
1:A:317:PHE:CD2	1:A:317:PHE:N	2.83	0.46
1:A:326:THR:HA	1:A:331:THR:HA	1.98	0.46
1:A:342:GLN:HG3	1:A:652:THR:HG22	1.98	0.46
1:A:342:GLN:HG3	1:A:652:THR:CG2	2.46	0.46
1:A:361:GLY:HA3	1:A:374:PRO:CG	2.40	0.46
1:A:555:LEU:C	1:A:555:LEU:CD2	2.84	0.46
1:A:270:ASP:HA	1:A:514:ARG:HG2	1.98	0.45
1:A:283:PHE:CZ	1:A:316:LEU:HD21	2.51	0.45
1:A:312:LEU:C	1:A:312:LEU:CD1	2.85	0.45
1:A:340:THR:HA	1:A:404:LEU:O	2.15	0.45
1:A:411:THR:CG2	1:A:412:PHE:N	2.79	0.45
1:A:316:LEU:HB2	1:A:410:PHE:HB3	1.98	0.45
1:A:396:LEU:HD23	1:A:396:LEU:N	2.31	0.45
1:A:528:LYS:HE3	1:A:575:GLU:OE1	2.15	0.45
1:A:701:TYR:CE1	1:A:727:ILE:HG13	2.52	0.45
1:A:230:CYS:SG	1:A:243:SER:HA	2.57	0.44
1:A:333:ILE:H	1:A:333:ILE:CD1	2.10	0.44
1:A:342:GLN:O	1:A:649:ILE:HA	2.17	0.44
1:A:247:TRP:CB	1:A:373:ILE:HD11	2.45	0.44
1:A:283:PHE:HB2	1:A:647:ILE:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LYS:HD2	1:A:686:GLU:HB2	2.00	0.44
1:A:287:ARG:C	1:A:618:ILE:HD11	2.37	0.44
1:A:530:ASP:O	1:A:531:LYS:CG	2.66	0.44
1:A:233:THR:O	1:A:239:VAL:HA	2.18	0.44
1:A:532:ASP:OD2	1:A:562:ASP:OD2	2.35	0.44
1:A:514:ARG:HE	1:A:514:ARG:HB2	1.51	0.43
1:A:343:VAL:HA	1:A:648:LEU:O	2.18	0.43
1:A:288:PHE:CD1	1:A:618:ILE:HD13	2.53	0.43
1:A:444:TYR:CE2	1:A:465:ARG:HB3	2.54	0.43
1:A:297:TRP:CZ2	1:A:729:THR:HG22	2.54	0.43
1:A:520:PRO:HA	1:A:538:SER:O	2.19	0.43
1:A:547:SER:OG	1:A:557:ASN:ND2	2.52	0.43
1:A:509:TYR:HB3	1:A:518:ILE:HD11	2.00	0.43
1:A:423:SER:HB2	1:A:425:TYR:CE2	2.55	0.42
1:A:448:ARG:NE	1:A:452:GLN:HG3	2.35	0.42
1:A:714:THR:HG23	1:A:715:VAL:O	2.20	0.42
1:A:272:HIS:HB3	1:A:384:GLY:O	2.20	0.42
1:A:328:ASP:HB2	1:A:330:VAL:HG22	2.00	0.42
1:A:321:VAL:HG11	1:A:339:SER:CB	2.50	0.42
1:A:722:THR:O	1:A:722:THR:HG23	2.20	0.42
1:A:486:GLN:OE1	1:A:539:GLY:N	2.53	0.41
1:A:555:LEU:O	1:A:558:VAL:HG22	2.21	0.41
1:A:404:LEU:HD12	1:A:404:LEU:N	2.35	0.41
1:A:727:ILE:HG22	1:A:728:GLY:O	2.20	0.41
1:A:364:PRO:HA	1:A:365:PRO:HD3	1.92	0.41
1:A:701:TYR:CD2	1:A:701:TYR:C	2.93	0.41
1:A:256:LEU:O	1:A:279:PRO:HG3	2.21	0.41
1:A:284:ASP:OD2	1:A:362:CYS:SG	2.76	0.41
1:A:690:GLU:HG2	1:A:692:SER:H	1.86	0.41
1:A:342:GLN:CG	1:A:652:THR:HG22	2.51	0.41
1:A:343:VAL:HG12	1:A:344:PHE:H	1.86	0.41
1:A:453:SER:HB3	1:A:454:GLY:H	1.52	0.41
1:A:438:LEU:C	1:A:439:ILE:HG13	2.42	0.41
1:A:503:TRP:CE3	1:A:517:ILE:HD11	2.56	0.41
1:A:305:TRP:CE3	1:A:690:GLU:HA	2.56	0.40
1:A:525:ALA:HB3	1:A:572:VAL:HA	2.03	0.40
1:A:366:PHE:CE2	1:A:368:ALA:HB3	2.56	0.40
1:A:465:ARG:O	1:A:466:GLY:C	2.60	0.40
1:A:717:ASN:ND2	1:A:717:ASN:H	2.19	0.40
1:A:278:THR:CG2	1:A:376:TYR:O	2.69	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	517/534 (97%)	470 (91%)	42 (8%)	5 (1%)	15	53

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	SER
1	A	532	ASP
1	A	556	ASP
1	A	504	THR
1	A	466	GLY

### 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	452/460 (98%)	411 (91%)	41 (9%)	9	34

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	219	ASP
1	A	242	THR
1	A	244	THR
1	A	246	THR
1	A	278	THR
1	A	289	HIS

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Mol	Chain	Res	Type
1	A	312	LEU
1	A	313	ASN
1	A	319	ILE
1	A	323	GLU
1	A	324	VAL
1	A	325	THR
1	A	328	ASP
1	A	333	ILE
1	A	382	ASN
1	A	406	THR
1	A	412	PHE
1	A	413	SER
1	A	418	ASP
1	A	433	ARG
1	A	443	LEU
1	A	452	GLN
1	A	453	SER
1	A	479	LEU
1	A	483	CYS
1	A	489	VAL
1	A	493	LYS
1	A	532	ASP
1	A	564	GLU
1	A	575	GLU
1	A	576	ARG
1	A	589	THR
1	A	596	VAL
1	A	602	LEU
1	A	615	GLN
1	A	665	THR
1	A	678	GLN
1	A	690	GLU
1	A	691	ASN
1	A	714	THR
1	A	733	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	ASN
1	A	302	ASN
1	A	382	ASN

*Continued on next page...*

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Mol	Chain	Res	Type
1	A	402	GLN
1	A	429	GLN
1	A	447	ASN
1	A	487	GLN
1	A	498	ASN
1	A	500	ASN
1	A	510	ASN
1	A	552	ASN
1	A	557	ASN
1	A	615	GLN
1	A	678	GLN
1	A	691	ASN
1	A	704	ASN
1	A	717	ASN
1	A	718	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 ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

2 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	CYT	A	737	-	7,8,8	0.91	0	8,10,10	5.33	7 (87%)
3	OAH	A	999	-	21,24,24	1.12	1 (4%)	24,36,36	1.59	4 (16%)

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	CYT	A	737	-	-	-	0/1/1/1
3	OAH	A	999	-	-	1/6/22/22	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	OAH	P-O2P	3.51	1.61	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	737	CYT	C6-N1-C2	9.98	121.15	114.46
2	A	737	CYT	N3-C2-N1	-9.05	120.55	128.35
3	A	999	OAH	N3-C2-N1	-5.15	121.68	128.67
2	A	737	CYT	C4-N3-C2	4.34	120.74	116.34
2	A	737	CYT	C5-C6-N1	-3.29	119.94	123.97
3	A	999	OAH	O4'-C1'-C2'	-2.55	101.49	106.24
2	A	737	CYT	C6-C5-C4	2.42	118.25	116.90
2	A	737	CYT	N4-C4-N3	2.40	120.45	116.59
3	A	999	OAH	O3P-P-O5'	2.31	112.69	106.67
3	A	999	OAH	O4'-C1'-N9	2.06	111.48	108.75
2	A	737	CYT	C5-C4-N3	-2.04	119.37	121.83

There are no chirality outliers.

All (1) torsion outliers are listed below:

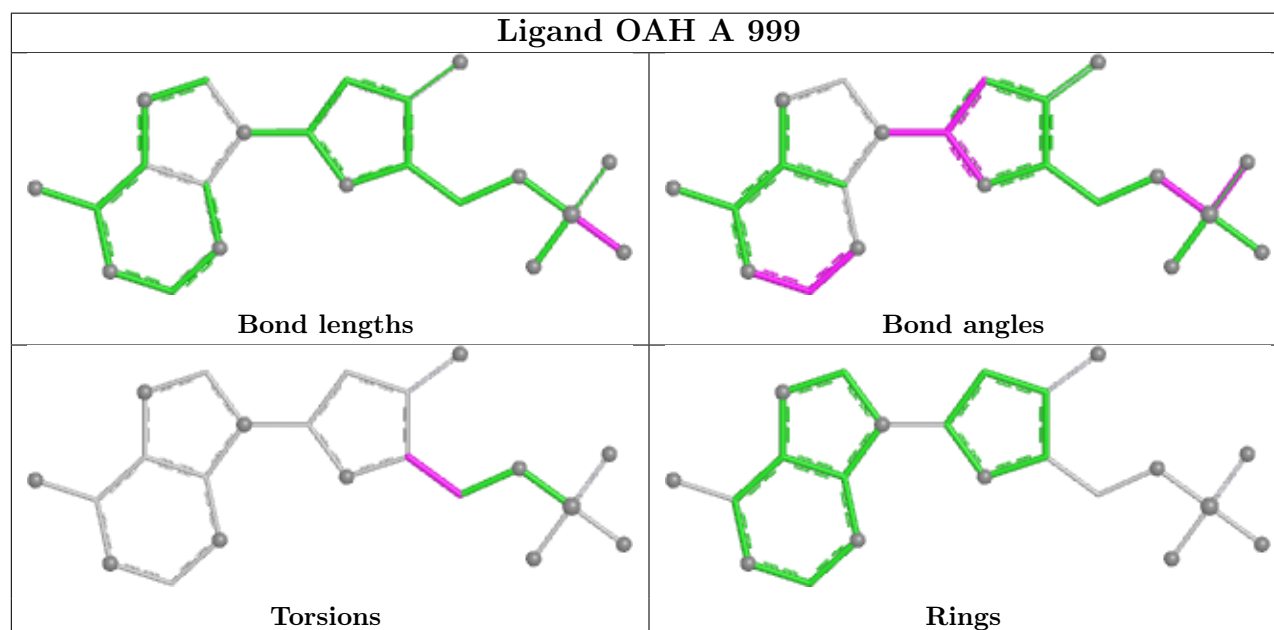
Mol	Chain	Res	Type	Atoms
3	A	999	OAH	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	OAH	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	519/534 (97%)	-0.15	14 (2%) 54 26	49, 60, 77, 110	3 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	328	ASP	4.3
1	A	453	SER	3.4
1	A	330	VAL	2.7
1	A	452	GLN	2.7
1	A	329	GLY	2.6
1	A	265	THR	2.5
1	A	454	GLY	2.5
1	A	415	THR	2.5
1	A	327	ASN	2.4
1	A	456	ALA	2.3
1	A	455	SER	2.3
1	A	218	ALA	2.3
1	A	499	SER	2.2
1	A	264	SER	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](#)

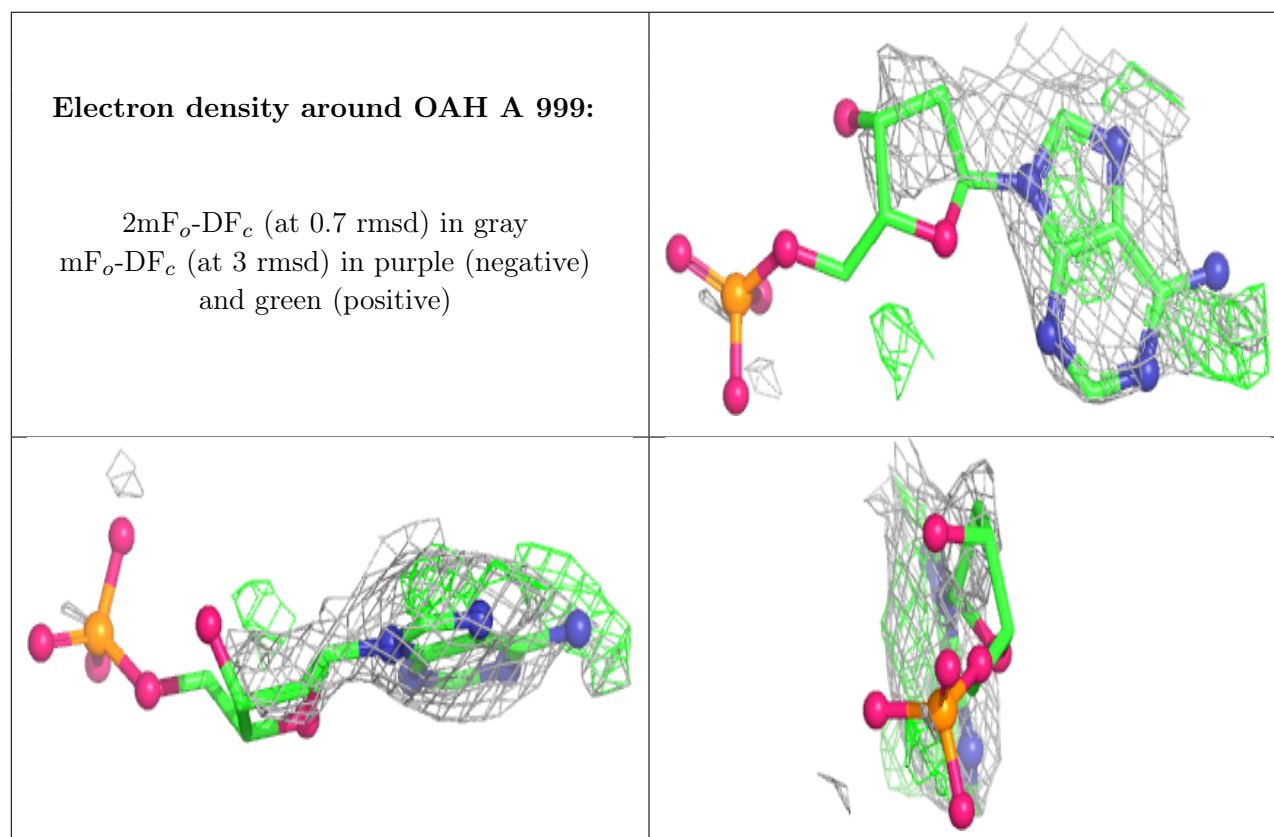
There are no monosaccharides in this entry.

## 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	OAH	A	999	22/22	0.47	0.60	76,82,94,94	22
2	CYT	A	737	8/8	0.85	0.28	42,44,45,45	8

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.