



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:31 AM UTC

PDB ID : 3OAH / pdb_00003oah
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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

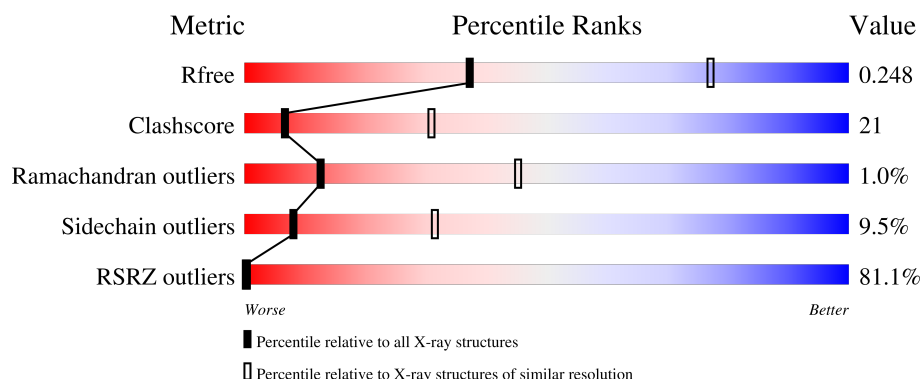
1 Overall quality at a glance

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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 ≥ 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	79% 58% 32% 6%

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	CYT	A	737	-	-	-	X

2 Entry composition [i](#)

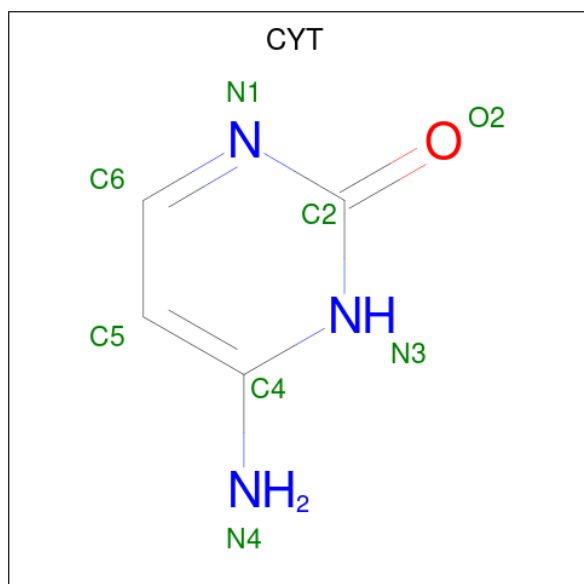
There are 4 unique types of molecules in this entry. The entry contains 4158 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

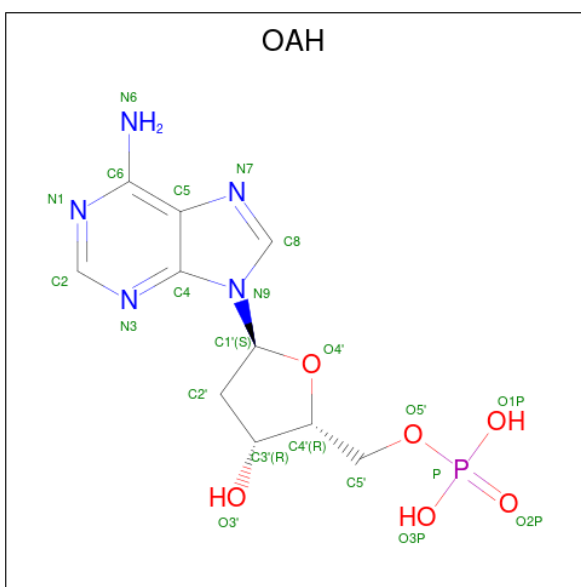
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	519	4117	2605	711	785	16	1	0	0

- Molecule 2 is 6-AMINOPYRIMIDIN-2(1H)-ONE (CCD ID: 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 (CCD ID: 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		

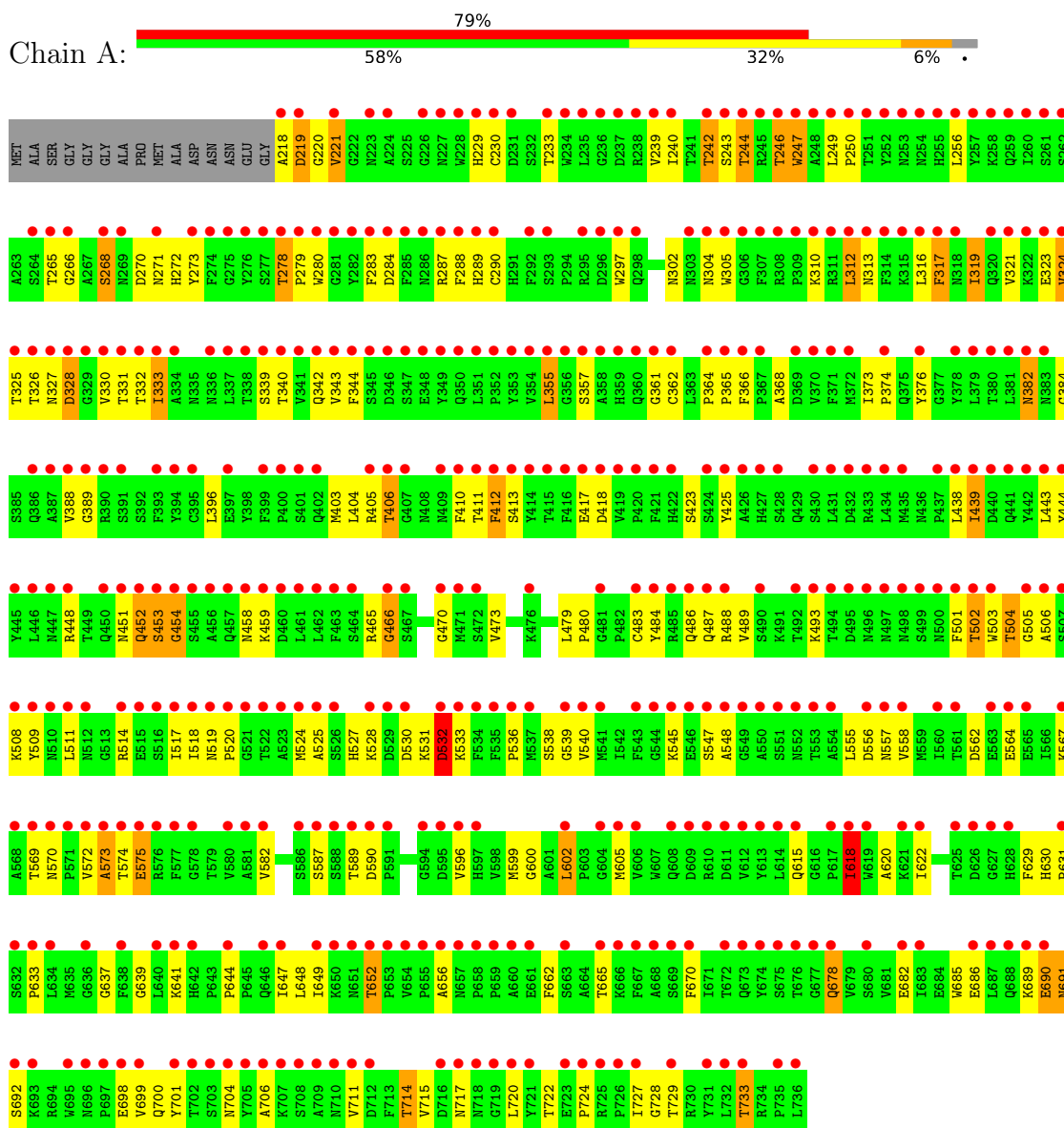
- Molecule 4 is water.

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, α , β , γ	263.00Å 263.00Å 609.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.00 40.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.00) 63.4 (40.00-3.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	50.1	Xtriage
Anisotropy	1.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.40	EDS
Total number of atoms	4158	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.54	1/4243 (0.0%)	1.03	22/5785 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	220	GLY	N-CA	5.34	1.48	1.44

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	GLY	N-CA-C	8.10	123.99	112.81
1	A	221	VAL	N-CA-C	-8.10	103.92	111.45
1	A	454	GLY	N-CA-C	-7.48	103.56	115.08
1	A	618	ILE	CB-CA-C	-6.93	105.82	111.71
1	A	573	ALA	N-CA-C	6.77	119.50	111.71
1	A	590	ASP	N-CA-C	6.22	117.64	109.93
1	A	656	ALA	N-CA-C	-6.21	102.49	110.19
1	A	545	LYS	N-CA-C	-6.03	102.99	110.41
1	A	357	SER	N-CA-C	-5.96	103.55	112.54
1	A	355	LEU	N-CA-C	-5.94	102.68	110.53
1	A	247	TRP	N-CA-C	5.89	118.80	110.14
1	A	439	ILE	N-CA-C	5.87	118.43	108.86
1	A	644	PRO	N-CA-C	-5.80	103.63	110.70
1	A	266	GLY	N-CA-C	-5.65	107.17	115.30
1	A	317	PHE	N-CA-C	5.62	117.34	108.96
1	A	662	PHE	N-CA-C	5.35	118.22	110.42
1	A	265	THR	N-CA-C	-5.32	106.80	113.72
1	A	670	PHE	N-CA-C	5.29	117.86	109.50
1	A	290	CYS	N-CA-C	-5.09	106.92	113.23
1	A	637	GLY	N-CA-C	5.02	118.10	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	652	THR	CA-C-N	5.01	124.94	119.78
1	A	652	THR	C-N-CA	5.01	124.94	119.78

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	173	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	173	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 21.

All (173) 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:602:LEU:HB2	1:A:605:MET:HE3	1.37	1.06
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:531:LYS:C	1:A:533:LYS:H	1.90	0.79
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:229:HIS:O	1:A:244:THR:HG22	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:527:HIS:HE2	1:A:532:ASP:CG	2.04	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:403:MET:C	1:A:404:LEU:HD12	2.21	0.65
1:A:691:ASN:HD22	1:A:691:ASN:C	2.05	0.64
1:A:247:TRP:HB2	1:A:373:ILE:CD1	2.28	0.64
1:A:555:LEU:HD23	1:A:555:LEU:C	2.23	0.64
1:A:629:PHE:O	1:A:630:HIS:C	2.41	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:312:LEU:C	1:A:312:LEU:HD12	2.24	0.61
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:324:VAL:HG23	1:A:331:THR:HG22	1.80	0.61
1:A:599:MET:HE3	1:A:600:GLY:H	1.66	0.61
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:711:VAL:O	1:A:714:THR:HB	2.03	0.59
1:A:555:LEU:HD23	1:A:555:LEU:O	2.03	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:531:LYS:C	1:A:533:LYS:N	2.61	0.58
1:A:691:ASN:C	1:A:691:ASN:ND2	2.59	0.58
1:A:297:TRP:HE1	1:A:727:ILE:HG22	1.69	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:319:ILE:C	1:A:319:ILE:HD12	2.32	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:527:HIS:NE2	1:A:532:ASP:CG	2.66	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:599:MET:HE3	1:A:600:GLY:N	2.23	0.52
1:A:328:ASP:C	1:A:330:VAL:H	2.16	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:273:TYR:C	1:A:273:TYR:CD1	2.88	0.51
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: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:555:LEU:C	1:A:555:LEU:CD2	2.84	0.50
1:A:280:TRP:NE1	1:A:396:LEU:HB2	2.27	0.50
1:A:312:LEU:C	1:A:312:LEU:CD1	2.85	0.50
1:A:582:VAL:HG12	1:A:582:VAL:O	2.11	0.49
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
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:287:ARG:C	1:A:618:ILE:HD11	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:GLY:O	1:A:473:VAL:HG12	2.12	0.48
1:A:403:MET:HE3	1:A:652:THR:HG21	1.95	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: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: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: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:701:TYR:CD2	1:A:701:TYR:C	2.93	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:438:LEU:C	1:A:439:ILE:HG13	2.42	0.45
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: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:465:ARG:O	1:A:466:GLY:C	2.60	0.45
1:A:528:LYS:HE3	1:A:575:GLU:OE1	2.15	0.45
1:A:600:GLY:O	1:A:605:MET:HE1	2.17	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
1:A:310:LYS:HD2	1:A:686:GLU:HB2	2.00	0.44
1:A:451:ASN:OD1	1:A:451:ASN:C	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:218:ALA:HB1	1:A:219:ASP:CG	2.43	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:256:LEU:C	1:A:279:PRO:HG3	2.44	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:405:ARG:O	1:A:406:THR:C	2.62	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:699:VAL:C	1:A:700:GLN:HG2	2.45	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: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:484:TYR:O	1:A:524:MET:HE1	2.20	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: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
1:A:555:LEU:C	1:A:557:ASN:H	2.29	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	517/534 (97%)	470 (91%)	42 (8%)	5 (1%)	12	45

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 [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	452/460 (98%)	409 (90%)	43 (10%)	8	31

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	219	ASP
1	A	221	VAL
1	A	242	THR
1	A	244	THR
1	A	246	THR
1	A	278	THR

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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	332	THR
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	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	502	THR
1	A	511	LEU
1	A	532	ASP
1	A	575	GLU
1	A	589	THR
1	A	596	VAL
1	A	602	LEU
1	A	615	GLN
1	A	618	ILE
1	A	665	THR
1	A	678	GLN
1	A	690	GLU
1	A	691	ASN
1	A	714	THR
1	A	720	LEU
1	A	733	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	ASN

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Mol	Chain	Res	Type
1	A	302	ASN
1	A	336	ASN
1	A	382	ASN
1	A	402	GLN
1	A	429	GLN
1	A	457	GLN
1	A	487	GLN
1	A	498	ASN
1	A	500	ASN
1	A	552	ASN
1	A	557	ASN
1	A	615	GLN
1	A	673	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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	OAH	A	999	-	24,24,24	1.34	4 (16%)	35,36,36	2.00	10 (28%)
2	CYT	A	737	-	7,8,8	2.55	2 (28%)	7,10,10	2.99	3 (42%)

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	OAH	A	999	-	-	3/10/22/22	0/3/3/3
2	CYT	A	737	-	-	-	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	737	CYT	O2-C2	6.10	1.36	1.24
3	A	999	OAH	P-O2P	3.51	1.61	1.50
3	A	999	OAH	C5-N7	-3.12	1.33	1.39
3	A	999	OAH	C8-N9	-2.29	1.33	1.37
3	A	999	OAH	C4-N9	-2.06	1.33	1.37
2	A	737	CYT	C2-N3	-2.05	1.34	1.39

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	737	CYT	C5-C6-N1	-6.07	119.94	124.75
3	A	999	OAH	C5-C4-N3	-5.25	119.48	126.72
3	A	999	OAH	N3-C2-N1	-4.56	121.68	128.58
2	A	737	CYT	C5-C4-N4	-3.81	120.17	123.88
3	A	999	OAH	N3-C4-N9	3.68	133.43	127.17
3	A	999	OAH	C2-N3-C4	3.56	120.53	111.83
3	A	999	OAH	N9-C8-N7	-3.03	109.64	113.94
3	A	999	OAH	C5-N7-C8	2.79	107.83	103.45
3	A	999	OAH	C4-C5-N7	-2.76	107.43	110.58
3	A	999	OAH	O4'-C1'-C2'	-2.55	101.49	106.25
2	A	737	CYT	C5-C4-N3	2.34	119.37	118.04
3	A	999	OAH	O3P-P-O5'	2.31	112.69	106.67
3	A	999	OAH	C4-N9-C8	2.16	108.01	105.74

There are no chirality outliers.

All (3) torsion outliers are listed below:

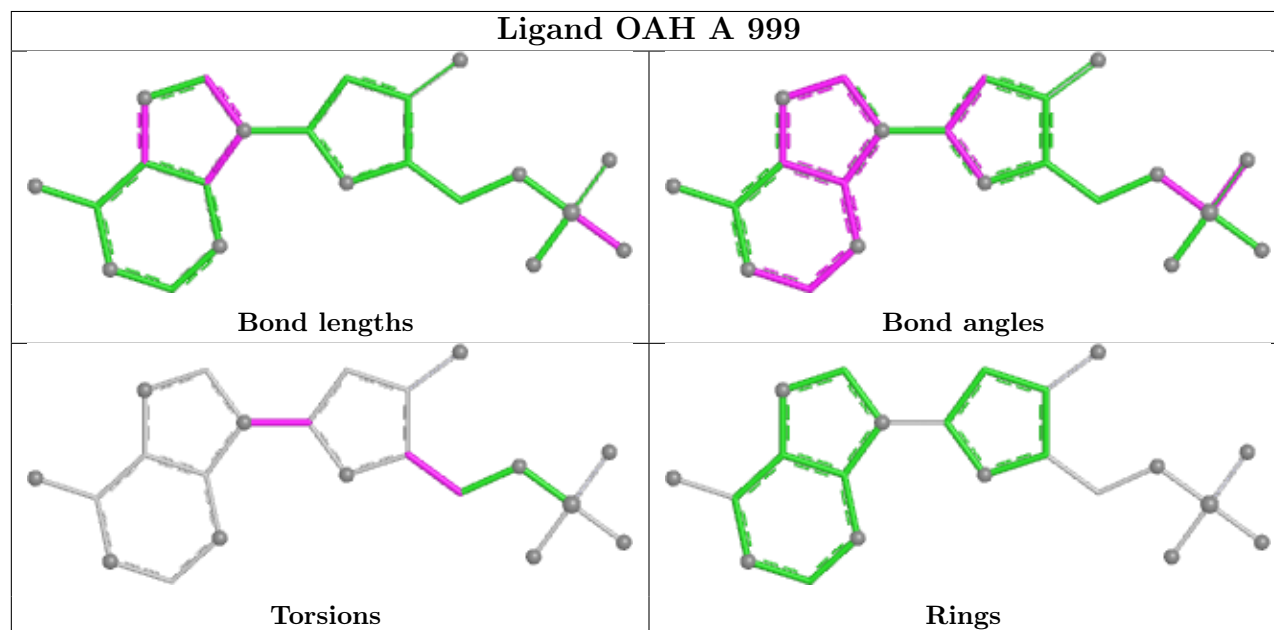
Mol	Chain	Res	Type	Atoms
3	A	999	OAH	O4'-C1'-N9-C4
3	A	999	OAH	O4'-C1'-N9-C8
3	A	999	OAH	O4'-C4'-C5'-O5'

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

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	519/534 (97%)	3.02	421 (81%) 0 0	27, 60, 77, 110	3 (0%)

All (421) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	328	ASP	10.5
1	A	229	HIS	8.7
1	A	327	ASN	7.9
1	A	281	GLY	7.8
1	A	456	ALA	7.0
1	A	331	THR	6.6
1	A	677	GLY	6.4
1	A	547	SER	6.4
1	A	704	ASN	6.1
1	A	452	GLN	6.0
1	A	455	SER	5.9
1	A	323	GLU	5.8
1	A	539	GLY	5.8
1	A	353	TYR	5.8
1	A	718	ASN	5.6
1	A	369	ASP	5.6
1	A	457	GLN	5.6
1	A	265	THR	5.6
1	A	530	ASP	5.5
1	A	370	VAL	5.4
1	A	705	TYR	5.4
1	A	352	PRO	5.4
1	A	549	GLY	5.2
1	A	401	SER	5.2
1	A	676	THR	5.2
1	A	389	GLY	5.2
1	A	522	THR	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	440	ASP	5.1
1	A	496	ASN	5.0
1	A	528	LYS	5.0
1	A	551	SER	5.0
1	A	448	ARG	4.9
1	A	400	PRO	4.9
1	A	702	THR	4.9
1	A	517	ILE	4.8
1	A	354	VAL	4.8
1	A	545	LYS	4.8
1	A	515	GLU	4.8
1	A	233	THR	4.8
1	A	356	GLY	4.7
1	A	660	ALA	4.7
1	A	471	MET	4.7
1	A	458	ASN	4.7
1	A	663	SER	4.6
1	A	246	THR	4.6
1	A	443	LEU	4.6
1	A	534	PHE	4.6
1	A	719	GLY	4.5
1	A	433	ARG	4.5
1	A	556	ASP	4.5
1	A	453	SER	4.4
1	A	590	ASP	4.4
1	A	360	GLN	4.4
1	A	422	HIS	4.4
1	A	244	THR	4.4
1	A	418	ASP	4.4
1	A	483	CYS	4.4
1	A	499	SER	4.4
1	A	230	CYS	4.3
1	A	711	VAL	4.3
1	A	340	THR	4.3
1	A	459	LYS	4.3
1	A	667	PHE	4.3
1	A	252	TYR	4.3
1	A	337	LEU	4.3
1	A	587	SER	4.3
1	A	237	ASP	4.2
1	A	493	LYS	4.2
1	A	321	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	731	TYR	4.2
1	A	318	ASN	4.1
1	A	510	ASN	4.1
1	A	546	GLU	4.1
1	A	641	LYS	4.1
1	A	569	THR	4.1
1	A	240	ILE	4.1
1	A	678	GLN	4.1
1	A	386	GLN	4.1
1	A	311	ARG	4.1
1	A	258	LYS	4.0
1	A	501	PHE	4.0
1	A	397	GLU	4.0
1	A	355	LEU	4.0
1	A	495	ASP	4.0
1	A	333	ILE	4.0
1	A	406	THR	4.0
1	A	249	LEU	4.0
1	A	261	SER	4.0
1	A	550	ALA	4.0
1	A	628	HIS	4.0
1	A	338	THR	4.0
1	A	588	SER	4.0
1	A	508	LYS	3.9
1	A	257	TYR	3.9
1	A	282	TYR	3.9
1	A	409	ASN	3.9
1	A	312	LEU	3.9
1	A	362	CYS	3.9
1	A	668	ALA	3.9
1	A	284	ASP	3.9
1	A	526	SER	3.9
1	A	461	LEU	3.9
1	A	361	GLY	3.9
1	A	673	GLN	3.9
1	A	431	LEU	3.9
1	A	470	GLY	3.8
1	A	428	SER	3.8
1	A	680	SER	3.8
1	A	413	SER	3.8
1	A	581	ALA	3.8
1	A	699	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	219	ASP	3.8
1	A	529	ASP	3.8
1	A	306	GLY	3.8
1	A	264	SER	3.8
1	A	445	TYR	3.8
1	A	594	GLY	3.8
1	A	570	ASN	3.7
1	A	293	SER	3.7
1	A	305	TRP	3.7
1	A	472	SER	3.7
1	A	669	SER	3.7
1	A	682	GLU	3.7
1	A	329	GLY	3.7
1	A	720	LEU	3.7
1	A	380	THR	3.7
1	A	514	ARG	3.7
1	A	260	ILE	3.7
1	A	582	VAL	3.7
1	A	608	GLN	3.7
1	A	227	ASN	3.7
1	A	387	ALA	3.6
1	A	706	ALA	3.6
1	A	245	ARG	3.6
1	A	577	PHE	3.6
1	A	736	LEU	3.6
1	A	399	PHE	3.6
1	A	638	PHE	3.6
1	A	228	TRP	3.6
1	A	500	ASN	3.6
1	A	697	PRO	3.6
1	A	326	THR	3.6
1	A	330	VAL	3.6
1	A	251	THR	3.6
1	A	341	VAL	3.6
1	A	696	ASN	3.6
1	A	276	TYR	3.6
1	A	414	TYR	3.6
1	A	503	TRP	3.5
1	A	511	LEU	3.5
1	A	507	SER	3.5
1	A	665	THR	3.5
1	A	388	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	709	ALA	3.5
1	A	372	MET	3.5
1	A	492	THR	3.5
1	A	675	SER	3.5
1	A	655	PRO	3.5
1	A	451	ASN	3.5
1	A	221	VAL	3.5
1	A	595	ASP	3.5
1	A	390	ARG	3.5
1	A	309	PRO	3.5
1	A	421	PHE	3.4
1	A	505	GLY	3.4
1	A	460	ASP	3.4
1	A	411	THR	3.4
1	A	450	GLN	3.4
1	A	611	ASP	3.4
1	A	274	PHE	3.4
1	A	565	GLU	3.4
1	A	509	TYR	3.4
1	A	342	GLN	3.4
1	A	432	ASP	3.4
1	A	651	ASN	3.4
1	A	283	PHE	3.4
1	A	654	VAL	3.4
1	A	516	SER	3.3
1	A	703	SER	3.3
1	A	365	PRO	3.3
1	A	615	GLN	3.3
1	A	670	PHE	3.3
1	A	324	VAL	3.3
1	A	253	ASN	3.3
1	A	371	PHE	3.3
1	A	381	LEU	3.3
1	A	391	SER	3.3
1	A	633	PRO	3.3
1	A	725	ARG	3.3
1	A	701	TYR	3.3
1	A	652	THR	3.3
1	A	707	LYS	3.3
1	A	578	GLY	3.3
1	A	485	ARG	3.2
1	A	357	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	288	PHE	3.2
1	A	313	ASN	3.2
1	A	576	ARG	3.2
1	A	292	PHE	3.2
1	A	497	ASN	3.2
1	A	627	GLY	3.2
1	A	726	PRO	3.2
1	A	247	TRP	3.2
1	A	382	ASN	3.2
1	A	518	ILE	3.2
1	A	567	LYS	3.2
1	A	307	PHE	3.2
1	A	364	PRO	3.1
1	A	520	PRO	3.1
1	A	591	PRO	3.1
1	A	441	GLN	3.1
1	A	332	THR	3.1
1	A	494	THR	3.1
1	A	686	GLU	3.1
1	A	367	PRO	3.1
1	A	224	ALA	3.1
1	A	320	GLN	3.1
1	A	250	PRO	3.1
1	A	659	PRO	3.1
1	A	693	LYS	3.0
1	A	644	PRO	3.0
1	A	573	ALA	3.0
1	A	646	GLN	3.0
1	A	688	GLN	3.0
1	A	540	VAL	3.0
1	A	348	GLU	3.0
1	A	322	LYS	3.0
1	A	317	PHE	3.0
1	A	625	THR	3.0
1	A	727	ILE	3.0
1	A	617	PRO	3.0
1	A	358	ALA	3.0
1	A	548	ALA	3.0
1	A	568	ALA	3.0
1	A	402	GLN	3.0
1	A	303	ASN	3.0
1	A	304	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	653	PRO	3.0
1	A	394	TYR	3.0
1	A	359	HIS	3.0
1	A	254	ASN	3.0
1	A	420	PRO	2.9
1	A	563	GLU	2.9
1	A	343	VAL	2.9
1	A	544	GLY	2.9
1	A	597	HIS	2.9
1	A	286	ASN	2.9
1	A	552	ASN	2.9
1	A	710	ASN	2.9
1	A	315	LYS	2.9
1	A	289	HIS	2.9
1	A	486	GLN	2.9
1	A	723	GLU	2.9
1	A	262	SER	2.9
1	A	374	PRO	2.9
1	A	351	LEU	2.9
1	A	462	LEU	2.9
1	A	383	ASN	2.9
1	A	395	CYS	2.9
1	A	412	PHE	2.9
1	A	454	GLY	2.9
1	A	255	HIS	2.8
1	A	698	GLU	2.8
1	A	416	PHE	2.8
1	A	466	GLY	2.8
1	A	640	LEU	2.8
1	A	708	SER	2.8
1	A	553	THR	2.8
1	A	612	VAL	2.8
1	A	236	GLY	2.8
1	A	376	TYR	2.8
1	A	674	TYR	2.8
1	A	506	ALA	2.8
1	A	733	THR	2.8
1	A	269	ASN	2.8
1	A	424	SER	2.8
1	A	533	LYS	2.8
1	A	692	SER	2.8
1	A	614	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	280	TRP	2.8
1	A	560	ILE	2.8
1	A	484	TYR	2.8
1	A	248	ALA	2.8
1	A	571	PRO	2.8
1	A	235	LEU	2.8
1	A	521	GLY	2.7
1	A	231	ASP	2.7
1	A	557	ASN	2.7
1	A	689	LYS	2.7
1	A	296	ASP	2.7
1	A	447	ASN	2.7
1	A	498	ASN	2.7
1	A	393	PHE	2.7
1	A	463	PHE	2.7
1	A	226	GLY	2.7
1	A	575	GLU	2.7
1	A	427	HIS	2.7
1	A	379	LEU	2.7
1	A	657	ASN	2.7
1	A	649	ILE	2.6
1	A	417	GLU	2.6
1	A	532	ASP	2.6
1	A	437	PRO	2.6
1	A	502	THR	2.6
1	A	602	LEU	2.6
1	A	339	SER	2.6
1	A	278	THR	2.6
1	A	523	ALA	2.6
1	A	535	PHE	2.6
1	A	537	MET	2.6
1	A	716	ASP	2.6
1	A	407	GLY	2.6
1	A	717	ASN	2.6
1	A	310	LYS	2.6
1	A	621	LYS	2.6
1	A	647	ILE	2.6
1	A	346	ASP	2.6
1	A	690	GLU	2.6
1	A	666	LYS	2.6
1	A	325	THR	2.6
1	A	541	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	239	VAL	2.5
1	A	519	ASN	2.5
1	A	334	ALA	2.5
1	A	561	THR	2.5
1	A	481	GLY	2.5
1	A	554	ALA	2.5
1	A	297	TRP	2.5
1	A	543	PHE	2.5
1	A	442	TYR	2.5
1	A	634	LEU	2.5
1	A	298	GLN	2.5
1	A	712	ASP	2.5
1	A	344	PHE	2.5
1	A	366	PHE	2.5
1	A	316	LEU	2.5
1	A	277	SER	2.5
1	A	632	SER	2.5
1	A	622	ILE	2.5
1	A	287	ARG	2.5
1	A	405	ARG	2.5
1	A	275	GLY	2.5
1	A	619	TRP	2.4
1	A	687	LEU	2.4
1	A	524	MET	2.4
1	A	596	VAL	2.4
1	A	512	ASN	2.4
1	A	259	GLN	2.4
1	A	285	PHE	2.4
1	A	234	TRP	2.4
1	A	242	THR	2.4
1	A	223	ASN	2.4
1	A	609	ASP	2.4
1	A	467	SER	2.4
1	A	290	CYS	2.4
1	A	589	THR	2.3
1	A	336	ASN	2.3
1	A	683	ILE	2.3
1	A	487	GLN	2.3
1	A	243	SER	2.3
1	A	695	TRP	2.3
1	A	656	ALA	2.3
1	A	435	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	721	TYR	2.3
1	A	564	GLU	2.3
1	A	476	LYS	2.3
1	A	735	PRO	2.3
1	A	426	ALA	2.3
1	A	732	LEU	2.3
1	A	419	VAL	2.3
1	A	525	ALA	2.3
1	A	430	SER	2.3
1	A	350	GLN	2.3
1	A	558	VAL	2.3
1	A	580	VAL	2.3
1	A	279	PRO	2.3
1	A	439	ILE	2.3
1	A	347	SER	2.3
1	A	425	TYR	2.3
1	A	218	ALA	2.2
1	A	631	PRO	2.2
1	A	672	THR	2.2
1	A	271	ASN	2.2
1	A	661	GLU	2.2
1	A	438	LEU	2.2
1	A	604	GLY	2.2
1	A	410	PHE	2.2
1	A	308	ARG	2.2
1	A	574	THR	2.2
1	A	606	VAL	2.2
1	A	618	ILE	2.2
1	A	446	LEU	2.2
1	A	658	PRO	2.2
1	A	415	THR	2.2
1	A	349	TYR	2.2
1	A	464	SER	2.2
1	A	490	SER	2.2
1	A	605	MET	2.2
1	A	238	ARG	2.2
1	A	444	TYR	2.1
1	A	266	GLY	2.1
1	A	536	PRO	2.1
1	A	642	HIS	2.1
1	A	378	TYR	2.1
1	A	610	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	434	LEU	2.1
1	A	729	THR	2.1
1	A	724	PRO	2.1
1	A	488	ARG	2.1
1	A	613	TYR	2.1
1	A	636	GLY	2.1
1	A	650	LYS	2.1
1	A	295	ARG	2.1
1	A	268	SER	2.0
1	A	586	SER	2.0
1	A	626	ASP	2.0
1	A	572	VAL	2.0
1	A	345	SER	2.0
1	A	273	TYR	2.0
1	A	314	PHE	2.0
1	A	256	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

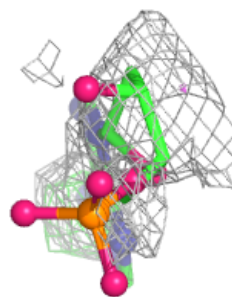
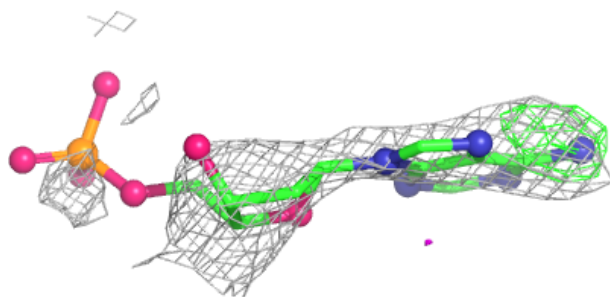
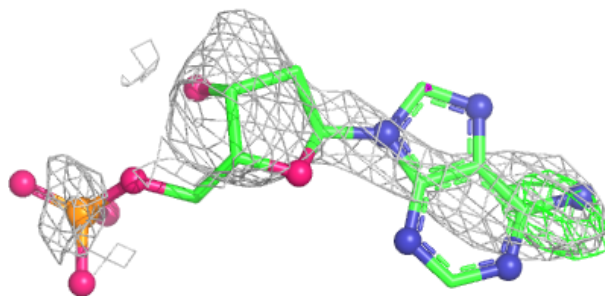
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CYT	A	737	8/8	0.65	0.41	42,44,45,45	8
3	OAH	A	999	22/22	0.80	0.38	76,82,94,94	22

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.

Electron density around OAH A 999:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.