



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:23 AM UTC

PDB ID : 2G8G / pdb_00002g8g
Title : Structurally mapping the diverse phenotype of Adeno-Associated Virus serotype 4
Authors : Govindasamy, L.; Padron, E.; McKenna, R.; Muzyczka, N.; Chiorini, J.A.; Agbandje-McKenna, M.
Deposited on : 2006-03-02
Resolution : 3.20 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

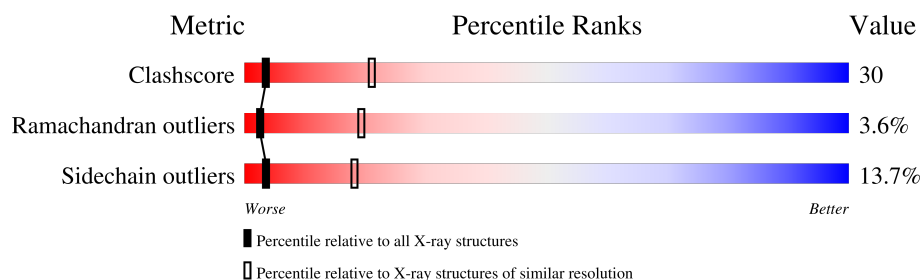
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	524	

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	D5M	A	21	X	-	-	-

2 Entry composition [i](#)

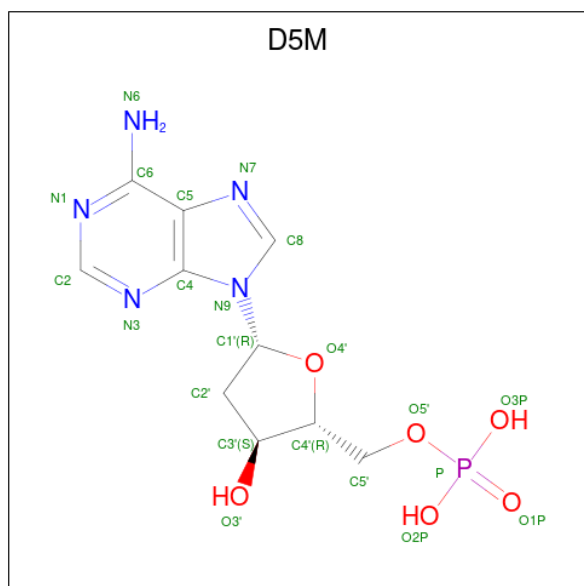
There are 3 unique types of molecules in this entry. The entry contains 4166 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	524	4129	2614	710	791	14	0	0	0

- Molecule 2 is 2'-DEOXYADENOSINE-5'-MONOPHOSPHATE (CCD ID: D5M) (formula: $C_{10}H_{14}N_5O_6P$).



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

- Molecule 3 is water.

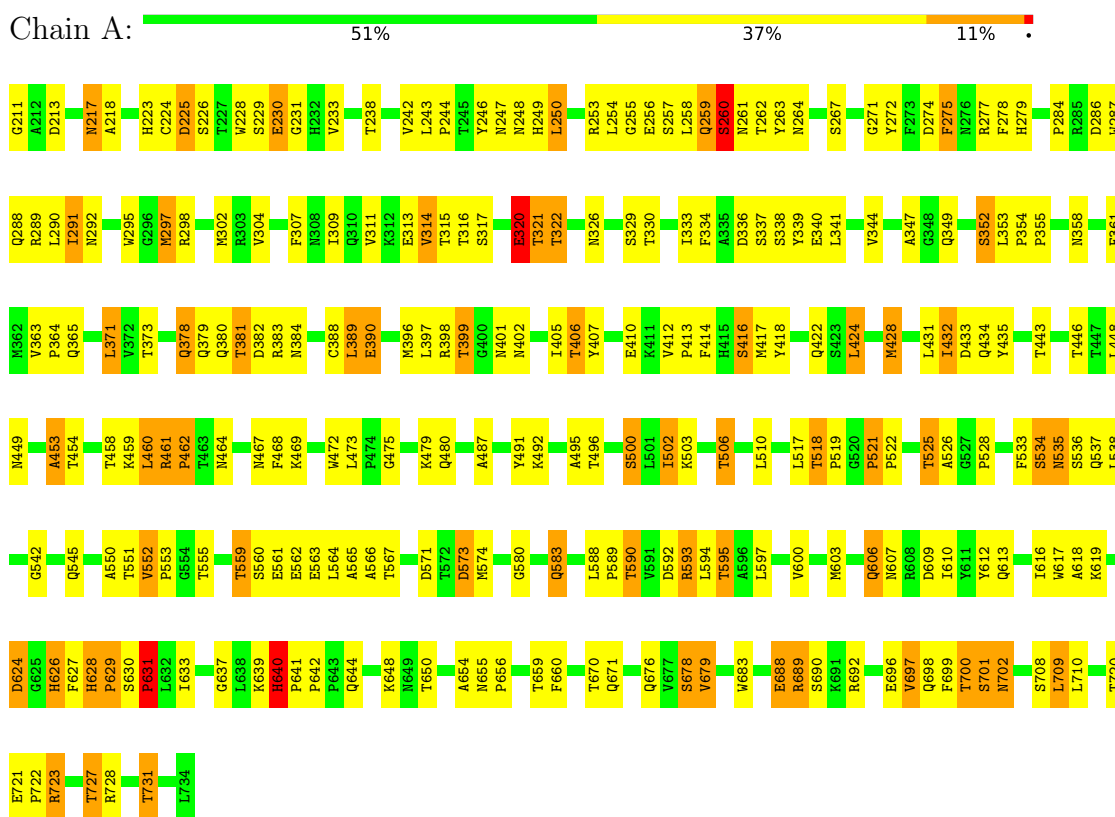
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	15	Total 15 O 15	0	0

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. 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. 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.

Note EDS was not executed.

• Molecule 1: Capsid



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	339.60 Å 319.20 Å 285.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.263 , 0.273	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4166	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: D5M

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	0.56	0/4259	1.12	29/5820 (0.5%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	475	GLY	CA-C-N	7.83	127.88	119.89
1	A	475	GLY	C-N-CA	7.83	127.88	119.89
1	A	660	PHE	N-CA-C	6.87	119.17	110.24
1	A	432	ILE	N-CA-C	6.69	119.77	108.86
1	A	435	TYR	N-CA-C	-6.45	104.57	112.88
1	A	434	GLN	N-CA-C	-6.44	102.23	110.53
1	A	250	LEU	N-CA-C	6.31	119.83	109.85
1	A	631	PRO	CA-N-CD	-6.27	103.23	112.00
1	A	286	ASP	CA-CB-CG	6.16	118.76	112.60
1	A	628	HIS	CA-C-N	6.06	127.41	119.84
1	A	628	HIS	C-N-CA	6.06	127.41	119.84
1	A	633	ILE	N-CA-C	-5.98	104.94	113.07
1	A	631	PRO	CB-CA-C	5.85	119.07	111.64
1	A	571	ASP	N-CA-C	5.84	118.15	111.02
1	A	671	GLN	N-CA-C	5.79	117.99	109.24
1	A	521	PRO	CB-CA-C	5.70	117.88	110.92
1	A	640	HIS	CA-C-N	5.70	126.25	120.38
1	A	640	HIS	C-N-CA	5.70	126.25	120.38
1	A	321	THR	N-CA-C	5.68	118.08	110.35
1	A	721	GLU	CA-C-N	5.40	126.59	119.84
1	A	721	GLU	C-N-CA	5.40	126.59	119.84
1	A	650	THR	CA-C-N	5.34	125.10	119.76
1	A	650	THR	C-N-CA	5.34	125.10	119.76
1	A	291	ILE	N-CA-C	5.33	120.31	113.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	ASN	N-CA-C	-5.30	105.46	112.94
1	A	338	SER	N-CA-C	-5.28	106.52	113.17
1	A	320	GLU	N-CA-C	5.23	118.25	110.14
1	A	378	GLN	N-CA-C	-5.17	106.94	113.20
1	A	307	PHE	N-CA-C	5.00	114.93	107.88

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	4129	0	3910	239	0
2	A	22	0	11	1	0
3	A	15	0	0	0	0
All	All	4166	0	3921	239	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 30.

All (239) 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:518:THR:CG2	1:A:519:PRO:HD3	1.74	1.16
1:A:518:THR:HB	1:A:519:PRO:HD2	1.26	1.08
1:A:518:THR:HG22	1:A:519:PRO:CD	1.86	1.05
1:A:518:THR:HG22	1:A:519:PRO:HD3	1.04	1.00
1:A:518:THR:CG2	1:A:519:PRO:CD	2.40	1.00
1:A:518:THR:CB	1:A:519:PRO:CD	2.43	0.96
1:A:518:THR:HB	1:A:519:PRO:CD	1.94	0.95
1:A:688:GLU:HG3	1:A:689:ARG:H	1.31	0.95
1:A:464:ASN:HD21	1:A:467:ASN:HD22	1.10	0.95
1:A:398:ARG:H	1:A:401:ASN:HD22	0.96	0.94
1:A:458:THR:HG22	1:A:460:LEU:H	1.29	0.94
1:A:417:MET:HA	1:A:727:THR:HG23	1.49	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:GLY:H	2:A:21:D5M:HN62	1.13	0.93
1:A:480:GLN:HA	1:A:506:THR:HG21	1.51	0.92
1:A:381:THR:HG22	1:A:382:ASP:H	1.34	0.91
1:A:607:ASN:HD21	1:A:628:HIS:HE1	1.18	0.89
1:A:518:THR:CB	1:A:519:PRO:HD2	2.03	0.88
1:A:600:VAL:HB	1:A:603:MET:HE3	1.59	0.84
1:A:304:VAL:HG22	1:A:679:VAL:HG13	1.59	0.82
1:A:398:ARG:N	1:A:401:ASN:HD22	1.75	0.81
1:A:230:GLU:HG3	1:A:231:GLY:H	1.45	0.81
1:A:609:ASP:OD1	1:A:727:THR:HG22	1.82	0.79
1:A:381:THR:H	1:A:384:ASN:ND2	1.81	0.78
1:A:381:THR:H	1:A:384:ASN:HD22	1.30	0.77
1:A:381:THR:N	1:A:384:ASN:HD22	1.84	0.76
1:A:223:HIS:NE2	1:A:225:ASP:CG	2.45	0.74
1:A:223:HIS:HE2	1:A:225:ASP:CG	1.94	0.74
1:A:538:LEU:O	1:A:559:THR:HB	1.88	0.73
1:A:464:ASN:ND2	1:A:467:ASN:HD22	1.86	0.73
1:A:309:ILE:O	1:A:399:THR:HG23	1.89	0.72
1:A:552:VAL:O	1:A:555:THR:HG22	1.89	0.72
1:A:257:SER:O	1:A:258:LEU:HD23	1.91	0.71
1:A:297:MET:HG2	1:A:417:MET:HE3	1.72	0.71
1:A:618:ALA:HB3	1:A:631:PRO:HG3	1.72	0.71
1:A:464:ASN:HD21	1:A:467:ASN:ND2	1.87	0.70
1:A:344:VAL:H	1:A:644:GLN:NE2	1.88	0.70
1:A:274:ASP:O	1:A:352:SER:HA	1.92	0.69
1:A:314:VAL:HG22	1:A:670:THR:HB	1.73	0.69
1:A:315:THR:O	1:A:322:THR:HG23	1.92	0.69
1:A:697:VAL:O	1:A:698:GLN:HG2	1.92	0.69
1:A:535:ASN:O	1:A:536:SER:HB2	1.92	0.68
1:A:259:GLN:O	1:A:260:SER:CB	2.42	0.68
1:A:480:GLN:HA	1:A:506:THR:CG2	2.24	0.68
1:A:259:GLN:O	1:A:260:SER:HB2	1.91	0.68
1:A:525:THR:HG23	1:A:526:ALA:N	2.10	0.67
1:A:618:ALA:HB3	1:A:631:PRO:CG	2.23	0.67
1:A:525:THR:CG2	1:A:561:GLU:H	2.08	0.66
1:A:292:ASN:ND2	1:A:698:GLN:HB3	2.12	0.65
1:A:257:SER:HA	1:A:262:THR:HG23	1.77	0.65
1:A:624:ASP:OD1	1:A:624:ASP:N	2.29	0.65
1:A:381:THR:HG22	1:A:382:ASP:N	2.11	0.64
1:A:480:GLN:OE1	1:A:506:THR:HG23	1.97	0.64
1:A:606:GLN:HA	1:A:606:GLN:HE21	1.61	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:ARG:NH1	1:A:731:THR:HG21	2.13	0.64
1:A:311:VAL:HG11	1:A:329:SER:HB3	1.80	0.63
1:A:396:MET:C	1:A:397:LEU:HD12	2.24	0.63
1:A:297:MET:HG2	1:A:417:MET:CE	2.29	0.63
1:A:278:PHE:CZ	1:A:610:ILE:HD11	2.34	0.63
1:A:284:PRO:HD3	1:A:612:TYR:OH	1.99	0.62
1:A:446:THR:HG22	1:A:446:THR:O	1.99	0.62
1:A:398:ARG:H	1:A:401:ASN:ND2	1.82	0.62
1:A:448:LEU:HD12	1:A:449:ASN:H	1.65	0.62
1:A:211:GLY:HA3	1:A:402:ASN:OD1	2.00	0.61
1:A:700:THR:CG2	1:A:701:SER:N	2.63	0.61
1:A:533:PHE:HA	1:A:537:GLN:HE22	1.66	0.61
1:A:279:HIS:CE1	1:A:355:PRO:HG3	2.35	0.60
1:A:347:ALA:HB3	1:A:349:GLN:HE21	1.66	0.60
1:A:292:ASN:HD22	1:A:698:GLN:HB3	1.65	0.60
1:A:458:THR:HG22	1:A:459:LYS:N	2.16	0.59
1:A:469:LYS:HD2	1:A:469:LYS:N	2.17	0.59
1:A:502:ILE:HG22	1:A:503:LYS:N	2.17	0.59
1:A:628:HIS:N	1:A:629:PRO:CD	2.65	0.59
1:A:248:ASN:O	1:A:249:HIS:HB2	2.01	0.59
1:A:688:GLU:O	1:A:689:ARG:HB2	2.01	0.59
1:A:295:TRP:CZ2	1:A:690:SER:HB3	2.38	0.58
1:A:295:TRP:HZ2	1:A:690:SER:HB3	1.69	0.58
1:A:358:ASN:CG	1:A:358:ASN:O	2.47	0.58
1:A:417:MET:HG2	1:A:727:THR:OG1	2.03	0.58
1:A:302:MET:HE1	1:A:642:PRO:HB3	1.85	0.58
1:A:627:PHE:C	1:A:629:PRO:HD3	2.28	0.58
1:A:688:GLU:HG3	1:A:689:ARG:N	2.08	0.58
1:A:534:SER:C	1:A:535:ASN:O	2.44	0.57
1:A:607:ASN:HD21	1:A:628:HIS:CE1	2.10	0.57
1:A:316:THR:HA	1:A:321:THR:HA	1.87	0.57
1:A:458:THR:HG22	1:A:460:LEU:N	2.11	0.57
1:A:709:LEU:HD23	1:A:710:LEU:H	1.69	0.57
1:A:626:HIS:CD2	1:A:629:PRO:HG3	2.40	0.57
1:A:278:PHE:CE1	1:A:616:ILE:HA	2.39	0.57
1:A:255:GLY:HA3	1:A:378:GLN:OE1	2.05	0.56
1:A:311:VAL:HG11	1:A:329:SER:CB	2.35	0.56
1:A:389:LEU:N	1:A:389:LEU:HD23	2.20	0.56
1:A:416:SER:O	1:A:417:MET:HB2	2.05	0.56
1:A:702:ASN:OD1	1:A:702:ASN:C	2.50	0.55
1:A:535:ASN:C	1:A:537:GLN:H	2.15	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:SER:O	1:A:230:GLU:C	2.50	0.54
1:A:564:LEU:HD22	1:A:606:GLN:HB3	1.89	0.54
1:A:263:TYR:CD1	1:A:263:TYR:C	2.86	0.54
1:A:275:PHE:CD2	1:A:679:VAL:HG21	2.43	0.54
1:A:550:ALA:HB1	1:A:555:THR:HG21	1.88	0.54
1:A:525:THR:HG22	1:A:561:GLU:H	1.72	0.54
1:A:259:GLN:O	1:A:259:GLN:HG3	2.08	0.54
1:A:320:GLU:HA	1:A:320:GLU:OE1	2.07	0.54
1:A:431:LEU:C	1:A:432:ILE:HG13	2.32	0.54
1:A:418:TYR:N	1:A:728:ARG:HG2	2.23	0.53
1:A:410:GLU:OE1	1:A:640:HIS:NE2	2.41	0.53
1:A:378:GLN:NE2	1:A:378:GLN:C	2.67	0.53
1:A:256:GLU:HG2	1:A:258:LEU:HD21	1.89	0.53
1:A:628:HIS:N	1:A:629:PRO:HD3	2.23	0.53
1:A:326:ASN:CG	1:A:329:SER:HB2	2.34	0.52
1:A:344:VAL:H	1:A:644:GLN:HE22	1.55	0.52
1:A:380:GLN:HB3	1:A:384:ASN:ND2	2.25	0.52
1:A:593:ARG:HH11	1:A:593:ARG:HG2	1.73	0.52
1:A:491:TYR:CG	1:A:491:TYR:O	2.63	0.52
1:A:559:THR:CG2	1:A:560:SER:N	2.73	0.51
1:A:491:TYR:O	1:A:491:TYR:CD2	2.64	0.51
1:A:443:THR:HA	1:A:453:ALA:HA	1.92	0.51
1:A:697:VAL:C	1:A:698:GLN:HG2	2.36	0.50
1:A:339:TYR:CE2	1:A:641:PRO:HD2	2.47	0.50
1:A:292:ASN:HB3	1:A:698:GLN:NE2	2.27	0.50
1:A:243:LEU:HD21	1:A:648:LYS:HA	1.92	0.50
1:A:317:SER:HB2	1:A:320:GLU:O	2.11	0.50
1:A:424:LEU:HD21	1:A:472:TRP:HB2	1.92	0.50
1:A:278:PHE:CZ	1:A:616:ILE:HG23	2.47	0.50
1:A:606:GLN:HE21	1:A:606:GLN:CA	2.22	0.50
1:A:290:LEU:CG	1:A:417:MET:HE1	2.42	0.49
1:A:378:GLN:HE21	1:A:379:GLN:N	2.09	0.49
1:A:458:THR:CG2	1:A:459:LYS:N	2.75	0.49
1:A:495:ALA:O	1:A:500:SER:HB3	2.11	0.49
1:A:433:ASP:OD2	1:A:461:ARG:HB3	2.12	0.49
1:A:583:GLN:HA	1:A:589:PRO:HD3	1.94	0.49
1:A:290:LEU:HD11	1:A:417:MET:HE1	1.95	0.49
1:A:528:PRO:HG3	1:A:560:SER:CB	2.43	0.49
1:A:313:GLU:O	1:A:313:GLU:HG3	2.11	0.49
1:A:257:SER:C	1:A:258:LEU:HD23	2.37	0.49
1:A:326:ASN:ND2	1:A:329:SER:HB2	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:THR:N	1:A:384:ASN:ND2	2.51	0.49
1:A:709:LEU:HD23	1:A:710:LEU:N	2.27	0.49
1:A:287:TRP:O	1:A:291:ILE:HG12	2.13	0.48
1:A:688:GLU:CG	1:A:689:ARG:H	2.12	0.48
1:A:593:ARG:HG2	1:A:593:ARG:NH1	2.29	0.48
1:A:460:LEU:HD22	1:A:468:PHE:HA	1.94	0.48
1:A:559:THR:HG23	1:A:560:SER:N	2.28	0.48
1:A:389:LEU:N	1:A:389:LEU:CD2	2.76	0.48
1:A:233:VAL:CG1	1:A:683:TRP:HB2	2.43	0.48
1:A:696:GLU:OE1	1:A:731:THR:HB	2.13	0.48
1:A:491:TYR:O	1:A:492:LYS:HB2	2.14	0.47
1:A:284:PRO:HD3	1:A:612:TYR:HH	1.78	0.47
1:A:479:LYS:CB	1:A:595:THR:HG23	2.44	0.47
1:A:230:GLU:HG3	1:A:231:GLY:N	2.24	0.47
1:A:418:TYR:H	1:A:728:ARG:HG2	1.80	0.47
1:A:580:GLY:HA3	1:A:590:THR:HG23	1.96	0.47
1:A:292:ASN:HD21	1:A:699:PHE:H	1.62	0.47
1:A:398:ARG:O	1:A:399:THR:C	2.56	0.47
1:A:630:SER:O	1:A:631:PRO:C	2.57	0.47
1:A:551:THR:HG22	1:A:551:THR:O	2.15	0.47
1:A:525:THR:HG23	1:A:526:ALA:O	2.15	0.47
1:A:688:GLU:O	1:A:689:ARG:CB	2.63	0.47
1:A:246:TYR:CE1	1:A:365:GLN:HB2	2.50	0.46
1:A:272:TYR:CE2	1:A:364:PRO:HB2	2.50	0.46
1:A:264:ASN:HB2	1:A:380:GLN:HE21	1.81	0.46
1:A:278:PHE:CD2	1:A:287:TRP:CZ3	3.03	0.46
1:A:340:GLU:O	1:A:341:LEU:HG	2.16	0.46
1:A:588:LEU:O	1:A:588:LEU:HD23	2.15	0.46
1:A:353:LEU:HD22	1:A:361:PHE:CZ	2.51	0.46
1:A:479:LYS:HB2	1:A:595:THR:HG23	1.96	0.46
1:A:371:LEU:HD23	1:A:371:LEU:O	2.16	0.46
1:A:274:ASP:OD2	1:A:274:ASP:C	2.59	0.46
1:A:641:PRO:O	1:A:642:PRO:C	2.57	0.46
1:A:277:ARG:NH1	1:A:613:GLN:O	2.42	0.45
1:A:388:CYS:SG	1:A:390:GLU:HG2	2.56	0.45
1:A:412:VAL:HG22	1:A:413:PRO:HD2	1.97	0.45
1:A:542:GLY:HA3	1:A:555:THR:O	2.17	0.45
1:A:616:ILE:HB	1:A:617:TRP:CE3	2.51	0.45
1:A:258:LEU:O	1:A:259:GLN:C	2.58	0.45
1:A:461:ARG:HB2	1:A:462:PRO:HD2	1.97	0.45
1:A:383:ARG:O	1:A:384:ASN:C	2.57	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:ASN:C	1:A:537:GLN:N	2.75	0.45
1:A:528:PRO:HG3	1:A:560:SER:HB3	1.99	0.45
1:A:246:TYR:CE1	1:A:365:GLN:HA	2.52	0.45
1:A:378:GLN:NE2	1:A:379:GLN:HA	2.32	0.45
1:A:479:LYS:O	1:A:506:THR:HG21	2.17	0.45
1:A:533:PHE:HA	1:A:537:GLN:NE2	2.30	0.45
1:A:243:LEU:HA	1:A:244:PRO:HD3	1.72	0.44
1:A:459:LYS:O	1:A:460:LEU:HB2	2.17	0.44
1:A:626:HIS:CD2	1:A:629:PRO:CG	3.00	0.44
1:A:254:LEU:HD11	1:A:267:SER:HB3	1.99	0.44
1:A:292:ASN:HD21	1:A:699:PHE:N	2.14	0.44
1:A:333:ILE:HG22	1:A:334:PHE:N	2.33	0.44
1:A:580:GLY:HA2	1:A:592:ASP:OD2	2.17	0.44
1:A:290:LEU:HG	1:A:417:MET:HE1	1.99	0.44
1:A:495:ALA:O	1:A:500:SER:CB	2.66	0.44
1:A:720:THR:O	1:A:722:PRO:HD3	2.17	0.44
1:A:449:ASN:CG	1:A:449:ASN:O	2.59	0.43
1:A:562:GLU:HG3	1:A:563:GLU:N	2.33	0.43
1:A:405:ILE:HG12	1:A:406:THR:N	2.34	0.43
1:A:606:GLN:HA	1:A:606:GLN:NE2	2.29	0.43
1:A:353:LEU:HD22	1:A:361:PHE:CE2	2.53	0.43
1:A:619:LYS:HB2	1:A:641:PRO:HG3	2.00	0.43
1:A:278:PHE:CE1	1:A:610:ILE:HD11	2.54	0.43
1:A:700:THR:HG22	1:A:701:SER:N	2.33	0.43
1:A:298:ARG:CZ	1:A:414:PHE:CE1	3.02	0.43
1:A:278:PHE:CD2	1:A:287:TRP:HZ3	2.36	0.43
1:A:288:GLN:O	1:A:289:ARG:C	2.61	0.43
1:A:525:THR:HB	1:A:561:GLU:HB2	2.00	0.43
1:A:428:MET:HG2	1:A:468:PHE:HD1	1.84	0.42
1:A:564:LEU:C	1:A:566:ALA:H	2.26	0.42
1:A:228:TRP:HH2	1:A:290:LEU:HB2	1.83	0.42
1:A:448:LEU:HD12	1:A:449:ASN:N	2.32	0.42
1:A:217:ASN:O	1:A:218:ALA:C	2.62	0.42
1:A:412:VAL:HA	1:A:413:PRO:HD3	1.93	0.42
1:A:460:LEU:HD21	1:A:467:ASN:O	2.19	0.42
1:A:552:VAL:O	1:A:553:PRO:C	2.62	0.42
1:A:292:ASN:HB3	1:A:698:GLN:HE22	1.85	0.42
1:A:410:GLU:OE1	1:A:640:HIS:CD2	2.72	0.42
1:A:271:GLY:HA2	1:A:364:PRO:O	2.19	0.42
1:A:238:THR:OG1	1:A:678:SER:HB3	2.19	0.42
1:A:336:ASP:OD1	1:A:341:LEU:HB2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:LYS:HG3	1:A:573:ASP:O	2.19	0.42
1:A:700:THR:HG23	1:A:701:SER:N	2.34	0.42
1:A:654:ALA:O	1:A:655:ASN:C	2.63	0.42
1:A:521:PRO:HA	1:A:522:PRO:HD2	1.94	0.41
1:A:534:SER:OG	1:A:535:ASN:O	2.38	0.41
1:A:574:MET:CE	1:A:593:ARG:HB3	2.50	0.41
1:A:710:LEU:HD23	1:A:710:LEU:HA	1.83	0.41
1:A:722:PRO:C	1:A:723:ARG:HG2	2.44	0.41
1:A:247:ASN:O	1:A:248:ASN:C	2.62	0.41
1:A:279:HIS:ND1	1:A:355:PRO:HG3	2.35	0.41
1:A:311:VAL:HG11	1:A:329:SER:OG	2.21	0.41
1:A:407:TYR:OH	1:A:641:PRO:HA	2.21	0.41
1:A:609:ASP:OD1	1:A:728:ARG:HG3	2.20	0.41
1:A:279:HIS:HD2	1:A:613:GLN:HB3	1.86	0.41
1:A:363:VAL:HA	1:A:364:PRO:HD3	1.91	0.41
1:A:480:GLN:NE2	1:A:517:LEU:O	2.52	0.41
1:A:432:ILE:HG22	1:A:433:ASP:N	2.36	0.41
1:A:626:HIS:HB2	1:A:627:PHE:H	1.69	0.40
1:A:410:GLU:OE2	1:A:639:LYS:N	2.54	0.40
1:A:290:LEU:CD1	1:A:417:MET:HE1	2.52	0.40
1:A:354:PRO:HA	1:A:355:PRO:HD3	1.97	0.40
1:A:600:VAL:O	1:A:603:MET:HG3	2.22	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	522/524 (100%)	443 (85%)	60 (12%)	19 (4%)	2 19

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	226	SER
1	A	230	GLU
1	A	487	ALA
1	A	518	THR
1	A	259	GLN
1	A	573	ASP
1	A	689	ARG
1	A	225	ASP
1	A	422	GLN
1	A	453	ALA
1	A	462	PRO
1	A	535	ASN
1	A	688	GLU
1	A	701	SER
1	A	260	SER
1	A	416	SER
1	A	496	THR
1	A	629	PRO
1	A	565	ALA

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	452/452 (100%)	390 (86%)	62 (14%)	3 18

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	213	ASP
1	A	217	ASN
1	A	224	CYS
1	A	242	VAL
1	A	250	LEU
1	A	253	ARG
1	A	260	SER
1	A	275	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	297	MET
1	A	314	VAL
1	A	320	GLU
1	A	322	THR
1	A	330	THR
1	A	337	SER
1	A	352	SER
1	A	371	LEU
1	A	373	THR
1	A	381	THR
1	A	389	LEU
1	A	390	GLU
1	A	399	THR
1	A	406	THR
1	A	424	LEU
1	A	428	MET
1	A	454	THR
1	A	460	LEU
1	A	461	ARG
1	A	473	LEU
1	A	500	SER
1	A	502	ILE
1	A	506	THR
1	A	510	LEU
1	A	525	THR
1	A	534	SER
1	A	545	GLN
1	A	552	VAL
1	A	559	THR
1	A	567	THR
1	A	583	GLN
1	A	590	THR
1	A	593	ARG
1	A	594	LEU
1	A	595	THR
1	A	597	LEU
1	A	606	GLN
1	A	624	ASP
1	A	626	HIS
1	A	631	PRO
1	A	640	HIS
1	A	656	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	659	THR
1	A	676	GLN
1	A	678	SER
1	A	679	VAL
1	A	697	VAL
1	A	700	THR
1	A	702	ASN
1	A	708	SER
1	A	709	LEU
1	A	723	ARG
1	A	727	THR
1	A	731	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	232	HIS
1	A	247	ASN
1	A	248	ASN
1	A	279	HIS
1	A	288	GLN
1	A	292	ASN
1	A	308	ASN
1	A	349	GLN
1	A	378	GLN
1	A	379	GLN
1	A	380	GLN
1	A	384	ASN
1	A	401	ASN
1	A	420	HIS
1	A	440	GLN
1	A	456	ASN
1	A	464	ASN
1	A	471	ASN
1	A	481	GLN
1	A	489	GLN
1	A	537	GLN
1	A	583	GLN
1	A	606	GLN
1	A	607	ASN
1	A	626	HIS
1	A	628	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	640	HIS
1	A	644	GLN
1	A	698	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	D5M	A	21	-	24,24,24	1.44	3 (12%)	35,36,36	2.29	12 (34%)

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	D5M	A	21	-	1/1/4/4	1/10/22/22	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	21	D5M	O4'-C4'	-3.41	1.37	1.45
2	A	21	D5M	C8-N9	-2.89	1.32	1.37
2	A	21	D5M	C5-N7	-2.71	1.34	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	21	D5M	O4'-C4'-C5'	5.43	126.74	109.33
2	A	21	D5M	N3-C2-N1	-4.93	121.12	128.58
2	A	21	D5M	C5-C4-N3	-4.88	119.99	126.72
2	A	21	D5M	O5'-C5'-C4'	4.40	123.97	108.99
2	A	21	D5M	C2-N3-C4	3.57	120.55	111.83
2	A	21	D5M	N3-C4-N9	3.16	132.53	127.17
2	A	21	D5M	C4-C5-N7	-2.77	107.41	110.58
2	A	21	D5M	O5'-P-O1P	2.77	113.93	106.44
2	A	21	D5M	C2'-C3'-C4'	-2.71	97.31	102.80
2	A	21	D5M	N9-C8-N7	-2.69	110.11	113.94
2	A	21	D5M	C5-N7-C8	2.55	107.45	103.45
2	A	21	D5M	O4'-C1'-N9	2.34	112.16	107.96

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	21	D5M	C4'

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	21	D5M	O4'-C4'-C5'-O5'

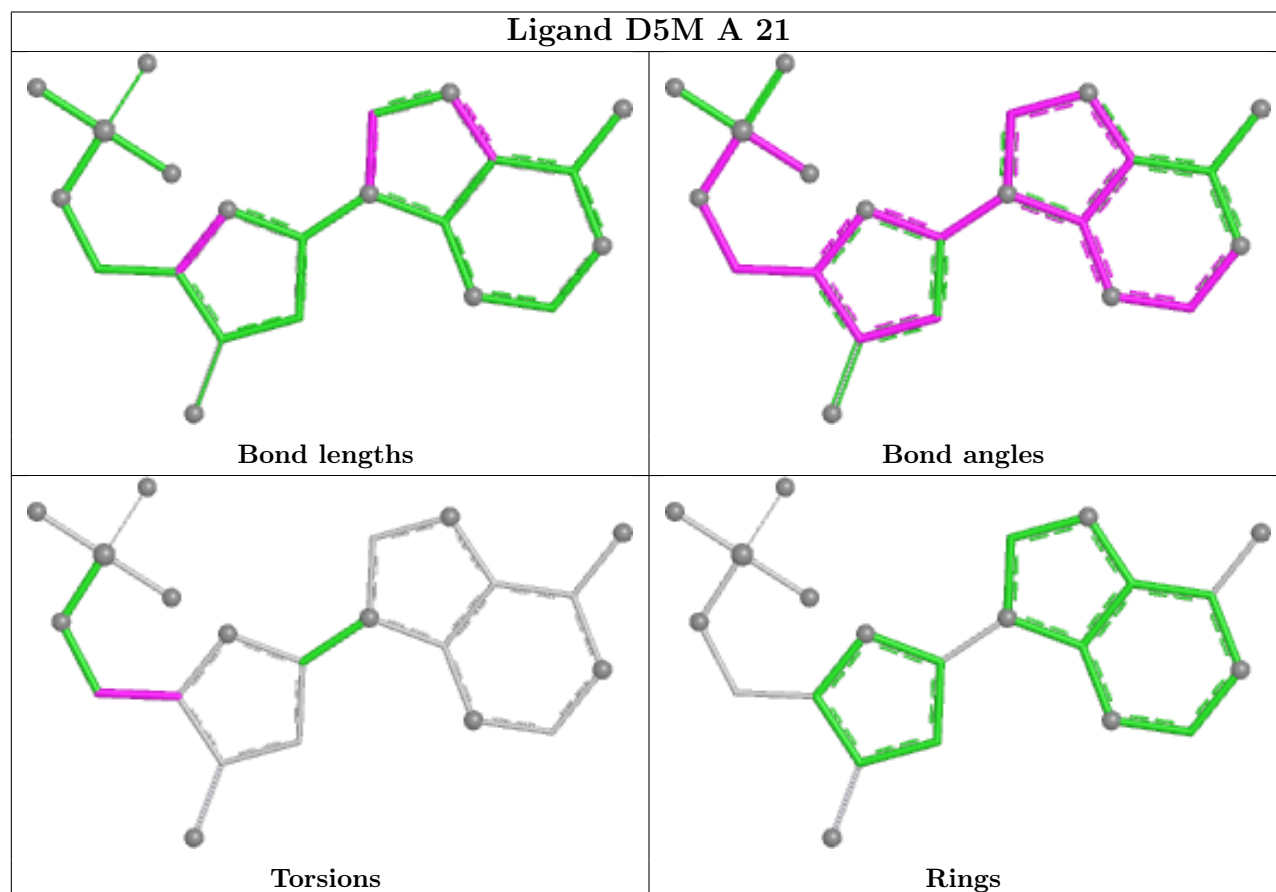
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	21	D5M	1	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.