



# Full wwPDB X-ray Structure Validation Report ⓘ

May 20, 2014 – 04:18 AM EDT

PDB ID : 4IOV  
Title : The structure of AAVrh32.33, a Novel Gene Delivery Vector  
Authors : Mikalim, K.; Nam, H.-J.; Van vilet, K.; Vandenberghe, L.H.; Mays, L.E.;  
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Deposited on : 2013-01-08  
Resolution : 3.50 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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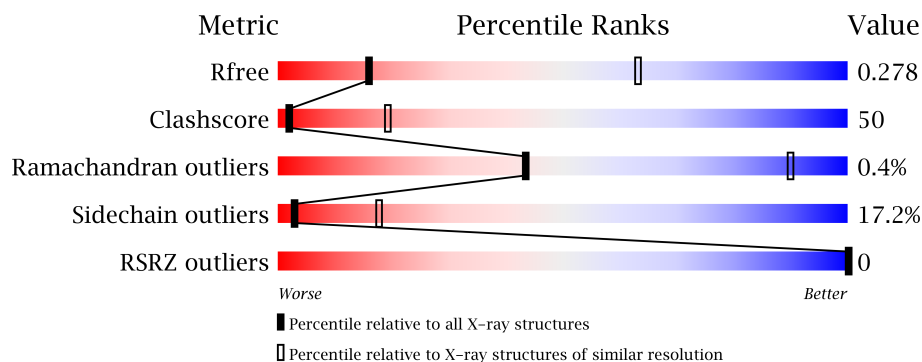
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable22978  
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) : stable22978

# 1 Overall quality at a glance

The reported resolution of this entry is 3.50 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	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)

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  $\geq 3$ , 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	733	

## 2 Entry composition i

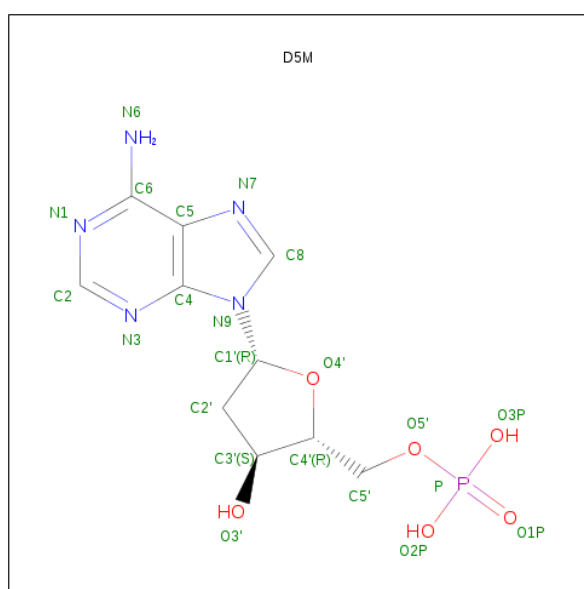
There are 2 unique types of molecules in this entry. The entry contains 4139 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	520	4117	2604	712	784	17	0	0	0

- Molecule 2 is 2'-DEOXYADENOSINE-5'-MONOPHOSPHATE (three-letter code: D5M) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>6</sub>P).



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	246.40Å 247.52Å 250.33Å 70.38° 65.37° 60.17°	Depositor
Resolution (Å)	40.00 – 3.50 31.14 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.50) 68.5 (31.14-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 3.47Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.271 , 0.269 0.277 , 0.278	Depositor DCC
$R_{free}$ test set	20013 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.7	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 10.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 396964 reflections	Xtriage
$F_o, F_c$ correlation	0.79	EDS
Total number of atoms	4139	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: 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	0.68	1/4245 (0.0%)	0.84	2/5798 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	628	PRO	C-N	-5.02	1.22	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	473	PRO	N-CA-C	5.33	125.95	112.10
1	A	452	ALA	N-CA-C	5.16	124.94	111.00

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	4117	0	3883	398	0
2	A	22	0	12	4	0
All	All	4139	0	3895	398	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 50.

All (398) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:253:ARG:C	1:A:254:LEU:HD23	1.23	1.51
1:A:253:ARG:O	1:A:254:LEU:CD2	1.90	1.18
1:A:507:TYR:CE2	1:A:514:SER:HB2	1.78	1.17
1:A:258:SER:O	1:A:262:THR:HG22	1.44	1.14
1:A:253:ARG:C	1:A:254:LEU:CD2	2.15	1.14
1:A:253:ARG:O	1:A:254:LEU:HD23	1.43	1.13
1:A:254:LEU:HD23	1:A:254:LEU:N	1.50	1.13
1:A:512:ARG:HH11	1:A:512:ARG:CB	1.64	1.10
1:A:512:ARG:HB2	1:A:512:ARG:HH11	1.17	1.04
1:A:268:THR:HG22	1:A:270:TRP:H	1.15	1.04
1:A:512:ARG:HH11	1:A:512:ARG:CG	1.70	1.04
1:A:257:THR:HG22	1:A:377:GLN:HG3	1.44	1.00
1:A:512:ARG:NH1	1:A:512:ARG:HB2	1.77	0.98
1:A:517:ALA:HB1	1:A:518:PRO:HD2	1.46	0.98
1:A:698:PHE:HB2	1:A:728:TYR:CE2	2.00	0.95
1:A:246:TYR:CE1	1:A:365:GLN:HB2	2.04	0.93
1:A:380:THR:H	1:A:383:ASN:HD22	1.15	0.92
1:A:627:HIS:HA	2:A:801:D5M:H2'1	1.52	0.92
1:A:648:ASN:HD22	1:A:648:ASN:N	1.64	0.92
1:A:687:GLU:HG3	1:A:688:ARG:H	1.35	0.92
1:A:347:ALA:O	1:A:349:GLN:HG3	1.71	0.90
1:A:344:VAL:H	1:A:643:GLN:NE2	1.71	0.89
1:A:344:VAL:H	1:A:643:GLN:HE22	1.19	0.89
1:A:563:ILE:HG22	1:A:567:ASN:OD1	1.73	0.88
1:A:338:SER:HB2	1:A:340:GLU:HG3	1.55	0.88
1:A:277:ARG:HH12	1:A:279:HIS:CE1	1.93	0.87
1:A:577:ILE:HD12	1:A:577:ILE:O	1.74	0.87
1:A:258:SER:O	1:A:262:THR:CG2	2.23	0.86
1:A:507:TYR:CE2	1:A:514:SER:CB	2.58	0.86
1:A:385:PHE:HD1	1:A:386:TYR:N	1.72	0.86
1:A:485:THR:OG1	1:A:488:GLN:HG2	1.75	0.86
1:A:567:ASN:HB2	1:A:568:PRO:HD2	1.59	0.84
1:A:618:LYS:HB2	1:A:640:PRO:HG3	1.58	0.84
1:A:277:ARG:NH1	1:A:279:HIS:CE1	2.45	0.83
1:A:292:ASN:HB3	1:A:697:GLN:HE21	1.42	0.81
1:A:262:THR:HG21	1:A:375:GLU:O	1.80	0.81
1:A:478:LYS:HE2	1:A:571:THR:O	1.79	0.81
1:A:345:MET:H	1:A:643:GLN:HE21	1.29	0.81
1:A:292:ASN:HD22	1:A:697:GLN:CG	1.94	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:292:ASN:HD22	1:A:697:GLN:HG2	1.44	0.80
1:A:415:SER:HB2	1:A:417:TYR:CE1	2.17	0.79
1:A:512:ARG:HH11	1:A:512:ARG:HG3	1.45	0.79
1:A:294:ASN:ND2	1:A:686:LYS:HD3	1.97	0.79
1:A:263:TYR:CD1	1:A:263:TYR:C	2.54	0.79
1:A:599:LEU:H	1:A:602:MET:HE3	1.47	0.79
1:A:713:ASP:OD1	1:A:715:THR:CG2	2.30	0.79
1:A:577:ILE:HD12	1:A:577:ILE:C	2.03	0.78
1:A:344:VAL:HG12	1:A:643:GLN:HE22	1.49	0.78
1:A:376:ASN:HD21	1:A:378:ASN:HD22	1.31	0.78
1:A:605:GLN:HE21	1:A:605:GLN:HA	1.49	0.77
1:A:380:THR:H	1:A:383:ASN:ND2	1.82	0.77
1:A:699:THR:HG23	1:A:699:THR:O	1.82	0.77
1:A:475:PRO:O	1:A:475:PRO:CD	2.30	0.76
1:A:575:GLY:O	1:A:593:VAL:HG12	1.83	0.76
1:A:243:LEU:HG	1:A:648:ASN:HD21	1.51	0.76
1:A:345:MET:H	1:A:643:GLN:NE2	1.82	0.76
1:A:567:ASN:CB	1:A:568:PRO:HD2	2.14	0.76
1:A:385:PHE:HD1	1:A:385:PHE:C	1.88	0.76
1:A:468:ARG:HD2	1:A:468:ARG:N	2.01	0.76
1:A:517:ALA:CB	1:A:518:PRO:HD2	2.15	0.76
1:A:616:TRP:CE2	1:A:641:PRO:HG2	2.20	0.76
1:A:517:ALA:HB1	1:A:518:PRO:CD	2.17	0.75
1:A:240:THR:HG23	1:A:675:GLN:OE1	1.86	0.75
1:A:648:ASN:H	1:A:648:ASN:HD22	1.34	0.75
1:A:713:ASP:OD1	1:A:715:THR:HG23	1.87	0.75
1:A:292:ASN:HD22	1:A:697:GLN:CB	1.99	0.74
1:A:292:ASN:HD21	1:A:698:PHE:H	1.33	0.74
1:A:304:VAL:HG22	1:A:678:VAL:HG22	1.68	0.74
1:A:309:ILE:O	1:A:398:THR:HG23	1.87	0.74
1:A:698:PHE:CZ	1:A:724:ILE:HD13	2.23	0.74
1:A:485:THR:OG1	1:A:488:GLN:CG	2.36	0.73
1:A:346:ASP:OD2	1:A:347:ALA:HB2	1.89	0.73
1:A:648:ASN:ND2	1:A:648:ASN:N	2.38	0.72
1:A:687:GLU:HG3	1:A:688:ARG:N	2.02	0.72
1:A:472:LEU:O	1:A:602:MET:HA	1.90	0.72
1:A:253:ARG:O	1:A:254:LEU:HD22	1.88	0.72
1:A:309:ILE:HG21	1:A:331:VAL:HG11	1.73	0.71
1:A:521:PRO:O	1:A:521:PRO:HG2	1.89	0.71
1:A:346:ASP:OD2	1:A:346:ASP:C	2.29	0.71
1:A:397:ARG:H	1:A:400:ASN:HD22	1.35	0.71
1:A:326:ASN:OD1	1:A:326:ASN:C	2.29	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:385:PHE:CD1	1:A:385:PHE:C	2.61	0.71
1:A:596:MET:HE3	1:A:596:MET:HA	1.72	0.71
1:A:515:ASN:OD1	1:A:515:ASN:C	2.30	0.70
1:A:292:ASN:HD22	1:A:697:GLN:HB3	1.57	0.70
1:A:700:SER:O	1:A:701:ASN:CG	2.30	0.70
1:A:299:PRO:HG2	1:A:408:PHE:HD2	1.57	0.70
1:A:380:THR:N	1:A:383:ASN:HD22	1.89	0.70
1:A:533:SER:H	1:A:536:GLN:NE2	1.88	0.69
1:A:512:ARG:NH1	1:A:512:ARG:HG3	2.02	0.69
1:A:577:ILE:HD13	1:A:578:ALA:O	1.93	0.69
1:A:713:ASP:C	1:A:713:ASP:OD1	2.30	0.69
1:A:285:ARG:HH11	1:A:288:GLN:HE21	1.40	0.69
1:A:701:ASN:OD1	1:A:701:ASN:C	2.30	0.69
1:A:290:LEU:HD21	1:A:297:LEU:HD13	1.75	0.69
1:A:599:LEU:H	1:A:602:MET:CE	2.05	0.68
1:A:599:LEU:N	1:A:602:MET:HE3	2.08	0.68
1:A:374:GLY:H	1:A:510:ASN:HD21	1.39	0.68
1:A:344:VAL:HG12	1:A:643:GLN:NE2	2.07	0.68
1:A:292:ASN:ND2	1:A:697:GLN:HB3	2.09	0.68
1:A:516:ILE:HG22	1:A:516:ILE:O	1.93	0.68
1:A:292:ASN:HD21	1:A:698:PHE:N	1.92	0.68
1:A:572:ASP:OD1	1:A:573:MET:N	2.27	0.68
1:A:432:ASP:OD2	1:A:460:ARG:HD2	1.94	0.68
1:A:533:SER:H	1:A:536:GLN:HE21	1.42	0.68
1:A:518:PRO:HG3	1:A:537:LEU:HD21	1.75	0.68
1:A:274:ASP:O	1:A:352:SER:HA	1.93	0.68
1:A:377:GLN:NE2	1:A:378:ASN:N	2.42	0.68
1:A:385:PHE:CD1	1:A:386:TYR:N	2.60	0.68
1:A:520:PRO:O	1:A:522:MET:HG3	1.93	0.67
1:A:346:ASP:OD2	1:A:347:ALA:N	2.28	0.67
1:A:459:ILE:CD1	1:A:468:ARG:HD3	2.25	0.67
1:A:475:PRO:O	1:A:475:PRO:CG	2.42	0.67
1:A:336:ASP:O	1:A:336:ASP:CG	2.34	0.66
1:A:377:GLN:C	1:A:377:GLN:NE2	2.48	0.66
1:A:704:ASN:HD22	1:A:704:ASN:N	1.93	0.66
1:A:246:TYR:CD1	1:A:365:GLN:HB2	2.30	0.66
1:A:334:PHE:CE1	1:A:645:PHE:HB2	2.30	0.66
1:A:380:THR:HG22	1:A:381:ASP:H	1.61	0.66
1:A:516:ILE:HG23	1:A:517:ALA:O	1.96	0.66
1:A:406:TYR:CE2	1:A:408:PHE:CD1	2.84	0.66
1:A:580:ASN:OD1	1:A:581:ASN:N	2.29	0.65
1:A:397:ARG:N	1:A:400:ASN:HD22	1.93	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:277:ARG:NH1	1:A:279:HIS:NE2	2.45	0.65
1:A:308:ASN:N	1:A:308:ASN:HD22	1.95	0.65
1:A:341:LEU:HD21	1:A:388:LEU:HD13	1.78	0.65
1:A:713:ASP:OD1	1:A:715:THR:N	2.30	0.65
1:A:654:ASN:OD1	1:A:655:PRO:N	2.30	0.64
1:A:447:LEU:HD12	1:A:447:LEU:O	1.95	0.64
1:A:344:VAL:N	1:A:643:GLN:HE22	1.93	0.64
1:A:699:THR:CG2	1:A:699:THR:O	2.45	0.64
1:A:406:TYR:HE2	1:A:408:PHE:CD1	2.16	0.64
1:A:222:TRP:CD1	1:A:222:TRP:O	2.52	0.63
1:A:222:TRP:O	1:A:222:TRP:HD1	1.81	0.63
1:A:608:ASP:OD1	1:A:609:ILE:N	2.32	0.62
1:A:294:ASN:OD1	1:A:684:ILE:HD12	1.99	0.62
1:A:257:THR:HG22	1:A:377:GLN:CG	2.24	0.62
1:A:316:THR:HG23	1:A:316:THR:O	1.98	0.62
1:A:713:ASP:OD1	1:A:715:THR:HG22	1.98	0.62
1:A:627:HIS:HA	2:A:801:D5M:C2'	2.26	0.62
1:A:268:THR:HB	1:A:366:TYR:O	1.99	0.62
1:A:222:TRP:CD1	1:A:222:TRP:C	2.73	0.61
1:A:314:VAL:CG1	1:A:669:THR:HB	2.30	0.61
1:A:464:PHE:HA	1:A:467:TYR:CD1	2.35	0.61
1:A:567:ASN:N	1:A:567:ASN:OD1	2.33	0.61
1:A:517:ALA:O	1:A:518:PRO:C	2.38	0.61
1:A:527:PRO:HG3	1:A:559:SER:HB3	1.82	0.61
1:A:314:VAL:HG13	1:A:669:THR:HB	1.83	0.61
1:A:700:SER:OG	1:A:701:ASN:N	2.32	0.61
1:A:475:PRO:O	1:A:475:PRO:HD2	1.99	0.60
1:A:617:ALA:HB3	1:A:630:PRO:HG3	1.82	0.60
1:A:480:GLN:HE21	1:A:481:ARG:H	1.49	0.60
1:A:277:ARG:HH12	1:A:279:HIS:HE1	1.50	0.60
1:A:315:THR:O	1:A:316:THR:HG22	2.02	0.60
1:A:292:ASN:ND2	1:A:697:GLN:HG2	2.17	0.59
1:A:654:ASN:OD1	1:A:655:PRO:HD2	2.01	0.59
1:A:507:TYR:HE2	1:A:514:SER:CB	2.12	0.59
1:A:268:THR:HG23	1:A:269:PRO:HD2	1.85	0.58
1:A:292:ASN:ND2	1:A:698:PHE:H	1.99	0.58
1:A:507:TYR:HD2	1:A:514:SER:O	1.87	0.58
1:A:713:ASP:OD2	1:A:715:THR:CG2	2.51	0.58
1:A:380:THR:HG22	1:A:381:ASP:N	2.17	0.58
1:A:713:ASP:CG	1:A:715:THR:CG2	2.72	0.58
1:A:432:ASP:N	1:A:432:ASP:OD1	2.35	0.58
1:A:654:ASN:OD1	1:A:655:PRO:CD	2.51	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:315:THR:HB	1:A:322:THR:HB	1.86	0.58
1:A:376:ASN:HD21	1:A:378:ASN:ND2	2.00	0.57
1:A:256:THR:O	1:A:256:THR:HG23	2.02	0.57
1:A:533:SER:HB3	1:A:570:ASP:OD2	2.05	0.57
1:A:608:ASP:HB2	1:A:727:ARG:NH1	2.18	0.57
1:A:538:ILE:N	1:A:538:ILE:HD12	2.19	0.57
1:A:517:ALA:CB	1:A:518:PRO:CD	2.81	0.57
1:A:406:TYR:CD1	1:A:642:PRO:HD3	2.39	0.57
1:A:311:VAL:HG11	1:A:329:SER:HB3	1.86	0.57
1:A:285:ARG:HH11	1:A:288:GLN:NE2	2.02	0.56
1:A:229:SER:HB2	1:A:232:LYS:O	2.05	0.56
1:A:292:ASN:HB3	1:A:697:GLN:NE2	2.17	0.56
1:A:285:ARG:NH1	1:A:288:GLN:NE2	2.54	0.56
1:A:345:MET:HE3	1:A:643:GLN:HA	1.86	0.56
1:A:256:THR:HG22	1:A:263:TYR:CE2	2.41	0.55
1:A:515:ASN:OD1	1:A:516:ILE:O	2.24	0.55
1:A:563:ILE:CG2	1:A:567:ASN:OD1	2.52	0.55
1:A:299:PRO:HB2	1:A:408:PHE:CE2	2.41	0.55
1:A:475:PRO:O	1:A:475:PRO:HG2	2.05	0.55
1:A:573:MET:SD	1:A:592:ASN:OD1	2.65	0.55
1:A:406:TYR:CE1	1:A:641:PRO:HA	2.42	0.55
1:A:423:LEU:HD23	1:A:423:LEU:C	2.26	0.55
1:A:510:ASN:O	1:A:511:ASN:HB2	2.05	0.55
1:A:507:TYR:CD2	1:A:514:SER:O	2.59	0.55
1:A:337:SER:O	1:A:339:TYR:CD1	2.60	0.55
1:A:478:LYS:CE	1:A:571:THR:O	2.54	0.55
1:A:599:LEU:N	1:A:602:MET:CE	2.66	0.55
1:A:713:ASP:CG	1:A:715:THR:HG22	2.27	0.55
1:A:275:PHE:CD2	1:A:678:VAL:HG21	2.42	0.55
1:A:577:ILE:CD1	1:A:578:ALA:O	2.55	0.55
1:A:374:GLY:N	1:A:510:ASN:HD21	2.03	0.54
1:A:577:ILE:HD12	1:A:578:ALA:C	2.27	0.54
1:A:257:THR:O	1:A:257:THR:OG1	2.23	0.54
1:A:519:GLY:O	1:A:520:PRO:C	2.45	0.54
1:A:356:PHE:HE2	1:A:358:ASN:HB3	1.71	0.54
1:A:272:TYR:O	1:A:364:PRO:HD2	2.07	0.54
1:A:395:MET:C	1:A:396:LEU:HD12	2.28	0.54
1:A:423:LEU:O	1:A:423:LEU:HD23	2.07	0.54
1:A:500:LEU:HD23	1:A:500:LEU:C	2.28	0.54
1:A:299:PRO:HG2	1:A:408:PHE:CD2	2.39	0.54
1:A:629:SER:O	1:A:630:PRO:C	2.45	0.53
1:A:627:HIS:CD2	2:A:801:D5M:H2'2	2.44	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:341:LEU:HD12	1:A:342:PRO:HD2	1.90	0.53
1:A:691:ARG:HH11	1:A:730:THR:HG21	1.72	0.53
1:A:292:ASN:ND2	1:A:697:GLN:CB	2.67	0.53
1:A:243:LEU:CG	1:A:648:ASN:HD21	2.19	0.53
1:A:659:PHE:CD1	1:A:660:THR:N	2.77	0.53
1:A:698:PHE:CZ	1:A:724:ILE:CD1	2.90	0.52
1:A:406:TYR:CD2	1:A:407:ASN:N	2.77	0.52
1:A:309:ILE:HG21	1:A:331:VAL:CG1	2.39	0.52
1:A:596:MET:HA	1:A:596:MET:CE	2.38	0.52
1:A:567:ASN:HB2	1:A:568:PRO:CD	2.37	0.52
1:A:302:MET:CE	1:A:641:PRO:HB3	2.40	0.52
1:A:515:ASN:OD1	1:A:516:ILE:N	2.43	0.52
1:A:632:ILE:HG22	1:A:632:ILE:O	2.09	0.52
1:A:563:ILE:HD11	1:A:727:ARG:NH1	2.25	0.52
1:A:353:LEU:HD22	1:A:361:PHE:CZ	2.45	0.52
1:A:304:VAL:HG22	1:A:678:VAL:CG2	2.38	0.52
1:A:599:LEU:HB2	1:A:602:MET:HE3	1.91	0.52
1:A:406:TYR:CD2	1:A:406:TYR:C	2.84	0.51
1:A:483:SER:HB3	1:A:488:GLN:HB2	1.90	0.51
1:A:555:LEU:C	1:A:556:LEU:HD23	2.31	0.51
1:A:432:ASP:HB3	1:A:461:SER:N	2.25	0.51
1:A:577:ILE:CD1	1:A:577:ILE:C	2.74	0.51
1:A:261:ASN:O	1:A:262:THR:C	2.48	0.51
1:A:263:TYR:HD1	1:A:264:ASN:N	2.09	0.51
1:A:257:THR:CG2	1:A:377:GLN:HG3	2.29	0.51
1:A:507:TYR:H	1:A:507:TYR:HD2	1.57	0.51
1:A:419:HIS:ND1	1:A:733:LEU:HD12	2.25	0.51
1:A:225:ASP:N	1:A:236:THR:O	2.42	0.51
1:A:237:SER:HB2	1:A:239:ARG:HH12	1.75	0.51
1:A:583:ASN:HB3	1:A:586:THR:OG1	2.11	0.51
1:A:334:PHE:HB3	1:A:393:SER:CB	2.41	0.50
1:A:299:PRO:CG	1:A:408:PHE:CD2	2.94	0.50
1:A:480:GLN:HG3	1:A:481:ARG:N	2.26	0.50
1:A:582:GLN:OE1	1:A:583:ASN:N	2.44	0.50
1:A:695:GLU:OE1	1:A:730:THR:HG22	2.10	0.50
1:A:523:ALA:HB3	1:A:569:ARG:HA	1.91	0.50
1:A:227:THR:O	1:A:227:THR:OG1	2.30	0.50
1:A:516:ILE:CG2	1:A:517:ALA:O	2.58	0.50
1:A:336:ASP:O	1:A:336:ASP:OD1	2.29	0.50
1:A:701:ASN:OD1	1:A:701:ASN:O	2.30	0.50
1:A:608:ASP:HB2	1:A:727:ARG:HH11	1.75	0.50
1:A:259:ASN:O	1:A:259:ASN:OD1	2.30	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:299:PRO:HB2	1:A:408:PHE:CD2	2.47	0.49
1:A:518:PRO:HB2	1:A:607:ARG:NH2	2.27	0.49
1:A:316:THR:HA	1:A:321:THR:HA	1.94	0.49
1:A:326:ASN:ND2	1:A:329:SER:HB2	2.26	0.49
1:A:309:ILE:CG2	1:A:331:VAL:HG11	2.42	0.49
1:A:700:SER:O	1:A:701:ASN:OD1	2.30	0.49
1:A:459:ILE:HD11	1:A:468:ARG:HD3	1.95	0.49
1:A:406:TYR:CE2	1:A:408:PHE:HD1	2.28	0.49
1:A:346:ASP:OD2	1:A:347:ALA:CB	2.59	0.49
1:A:377:GLN:HE21	1:A:378:ASN:N	2.10	0.49
1:A:396:LEU:HD12	1:A:396:LEU:N	2.27	0.49
1:A:294:ASN:HD21	1:A:686:LYS:HD3	1.74	0.49
1:A:326:ASN:OD1	1:A:326:ASN:O	2.30	0.49
1:A:257:THR:HB	1:A:377:GLN:H	1.78	0.48
1:A:307:PHE:N	1:A:307:PHE:CD1	2.81	0.48
1:A:346:ASP:HB2	1:A:617:ALA:HA	1.95	0.48
1:A:330:THR:OG1	1:A:330:THR:O	2.30	0.48
1:A:563:ILE:HD12	1:A:605:GLN:HB3	1.94	0.48
1:A:268:THR:HG22	1:A:269:PRO:N	2.29	0.48
1:A:345:MET:N	1:A:643:GLN:HE21	2.05	0.48
1:A:501:LEU:O	1:A:501:LEU:HD12	2.14	0.48
1:A:372:VAL:HG13	1:A:372:VAL:O	2.12	0.48
1:A:291:ILE:HD11	1:A:698:PHE:HD2	1.78	0.48
1:A:306:ILE:HD12	1:A:333:ILE:HD13	1.95	0.48
1:A:406:TYR:HD1	1:A:642:PRO:HD3	1.76	0.48
1:A:302:MET:HG2	1:A:303:ARG:N	2.28	0.48
1:A:388:LEU:CD2	1:A:388:LEU:N	2.77	0.47
1:A:432:ASP:CB	1:A:460:ARG:HA	2.44	0.47
1:A:330:THR:HA	1:A:396:LEU:O	2.14	0.47
1:A:537:LEU:C	1:A:538:ILE:HD12	2.35	0.47
1:A:599:LEU:CB	1:A:602:MET:HE3	2.44	0.47
1:A:247:ASN:O	1:A:248:ASN:C	2.52	0.47
1:A:388:LEU:HD22	1:A:388:LEU:N	2.29	0.47
1:A:356:PHE:CE2	1:A:358:ASN:HB3	2.50	0.47
1:A:298:ARG:NE	1:A:413:PHE:CE1	2.82	0.47
1:A:460:ARG:HH11	1:A:460:ARG:HG3	1.80	0.47
1:A:711:ALA:HB1	1:A:712:PRO:HD2	1.96	0.47
1:A:388:LEU:CD2	1:A:388:LEU:H	2.28	0.47
1:A:507:TYR:CD2	1:A:514:SER:HB2	2.45	0.47
1:A:570:ASP:OD1	1:A:571:THR:HG23	2.15	0.47
1:A:687:GLU:O	1:A:688:ARG:HB2	2.15	0.47
1:A:285:ARG:O	1:A:288:GLN:HB3	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:258:SER:C	1:A:262:THR:HG22	2.29	0.47
1:A:506:HIS:CD2	1:A:513:TRP:CD1	3.03	0.47
1:A:616:TRP:CZ2	1:A:641:PRO:HG2	2.49	0.47
1:A:263:TYR:HD1	1:A:263:TYR:C	2.14	0.46
1:A:500:LEU:HD21	1:A:504:ASP:OD2	2.16	0.46
1:A:567:ASN:CB	1:A:568:PRO:CD	2.90	0.46
1:A:236:THR:OG1	1:A:679:GLN:HG3	2.15	0.46
1:A:685:GLU:HG3	1:A:685:GLU:O	2.15	0.46
1:A:377:GLN:C	1:A:377:GLN:CD	2.74	0.46
1:A:435:LEU:HD12	1:A:468:ARG:HG3	1.98	0.46
1:A:640:PRO:O	1:A:641:PRO:C	2.51	0.46
1:A:702:TYR:CG	1:A:709:LEU:HD12	2.51	0.46
1:A:374:GLY:H	1:A:510:ASN:ND2	2.10	0.46
1:A:713:ASP:CG	1:A:715:THR:HG23	2.36	0.46
1:A:336:ASP:OD1	1:A:339:TYR:N	2.48	0.46
1:A:396:LEU:CD1	1:A:396:LEU:N	2.79	0.46
1:A:423:LEU:CD2	1:A:423:LEU:C	2.85	0.45
1:A:696:VAL:HG23	1:A:728:TYR:O	2.16	0.45
1:A:425:ARG:HA	1:A:427:MET:HE3	1.97	0.45
1:A:490:TYR:CD1	1:A:491:LYS:N	2.84	0.45
1:A:520:PRO:O	1:A:521:PRO:C	2.53	0.45
1:A:521:PRO:O	1:A:521:PRO:CG	2.55	0.45
1:A:295:TRP:O	1:A:416:MET:HB2	2.16	0.45
1:A:700:SER:HB2	1:A:702:TYR:CD2	2.51	0.45
1:A:605:GLN:NE2	1:A:605:GLN:HA	2.26	0.45
1:A:268:THR:CG2	1:A:269:PRO:N	2.80	0.45
1:A:379:GLN:HA	1:A:383:ASN:ND2	2.32	0.45
1:A:228:TRP:CE2	1:A:233:VAL:HG21	2.53	0.45
1:A:603:VAL:HG23	1:A:603:VAL:O	2.17	0.44
1:A:304:VAL:HG12	1:A:305:LYS:N	2.32	0.44
1:A:724:ILE:HG22	1:A:725:GLY:O	2.17	0.44
1:A:256:THR:O	1:A:256:THR:CG2	2.65	0.44
1:A:425:ARG:HE	1:A:425:ARG:HB3	1.46	0.44
1:A:577:ILE:CD1	1:A:578:ALA:C	2.86	0.43
1:A:263:TYR:O	1:A:263:TYR:CD1	2.71	0.43
1:A:297:LEU:HG	1:A:298:ARG:N	2.33	0.43
1:A:376:ASN:OD1	1:A:377:GLN:N	2.51	0.43
1:A:432:ASP:HB2	1:A:459:ILE:O	2.19	0.43
1:A:258:SER:O	1:A:262:THR:N	2.51	0.43
1:A:283:SER:O	1:A:284:PRO:C	2.56	0.43
1:A:377:GLN:C	1:A:377:GLN:HE21	2.22	0.43
1:A:333:ILE:HG12	1:A:646:ILE:HG13	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:308:ASN:N	1:A:308:ASN:ND2	2.64	0.43
1:A:636:GLY:H	2:A:801:D5M:HN62	1.67	0.43
1:A:387:CYS:SG	1:A:389:GLU:HG2	2.59	0.43
1:A:713:ASP:OD2	1:A:715:THR:HG22	2.19	0.43
1:A:338:SER:HB2	1:A:340:GLU:CG	2.36	0.43
1:A:343:TYR:CE1	1:A:643:GLN:HG3	2.54	0.43
1:A:409:GLU:HG2	1:A:409:GLU:H	1.54	0.43
1:A:512:ARG:NH1	1:A:512:ARG:CB	2.43	0.43
1:A:698:PHE:CE2	1:A:724:ILE:HD13	2.54	0.43
1:A:512:ARG:NH1	1:A:512:ARG:CG	2.41	0.42
1:A:561:GLU:HG3	1:A:561:GLU:H	1.52	0.42
1:A:583:ASN:OD1	1:A:584:ALA:N	2.52	0.42
1:A:698:PHE:HB2	1:A:728:TYR:CZ	2.49	0.42
1:A:229:SER:HB2	1:A:232:LYS:H	1.84	0.42
1:A:555:LEU:O	1:A:556:LEU:HD23	2.19	0.42
1:A:438:LEU:HB2	1:A:456:PHE:CE1	2.54	0.42
1:A:438:LEU:HD12	1:A:439:GLN:N	2.34	0.42
1:A:277:ARG:NH1	1:A:277:ARG:HG3	2.34	0.42
1:A:372:VAL:HG11	1:A:512:ARG:HE	1.84	0.42
1:A:599:LEU:HG	1:A:602:MET:CE	2.49	0.42
1:A:663:ARG:HD2	1:A:664:VAL:O	2.19	0.42
1:A:691:ARG:NH1	1:A:730:THR:HG21	2.33	0.42
1:A:460:ARG:NH1	1:A:460:ARG:HG3	2.34	0.42
1:A:268:THR:HG23	1:A:269:PRO:CD	2.50	0.42
1:A:277:ARG:CG	1:A:277:ARG:HH11	2.32	0.42
1:A:330:THR:O	1:A:649:THR:HB	2.19	0.42
1:A:371:ILE:O	1:A:371:ILE:HG23	2.18	0.42
1:A:425:ARG:HB3	1:A:427:MET:HE1	2.01	0.42
1:A:521:PRO:C	1:A:522:MET:HG3	2.39	0.42
1:A:582:GLN:OE1	1:A:582:GLN:C	2.57	0.42
1:A:298:ARG:CZ	1:A:413:PHE:HE1	2.32	0.42
1:A:509:LEU:O	1:A:512:ARG:NH1	2.53	0.42
1:A:574:PHE:HB3	1:A:593:VAL:HG13	2.01	0.42
1:A:605:GLN:HE21	1:A:605:GLN:CA	2.22	0.42
1:A:333:ILE:HG23	1:A:645:PHE:O	2.19	0.42
1:A:265:GLY:C	1:A:266:PHE:CD1	2.93	0.42
1:A:575:GLY:C	1:A:593:VAL:HG12	2.40	0.42
1:A:300:LYS:O	1:A:408:PHE:HB2	2.20	0.42
1:A:485:THR:OG1	1:A:488:GLN:HG3	2.16	0.42
1:A:302:MET:CG	1:A:303:ARG:N	2.83	0.41
1:A:414:HIS:CD2	1:A:609:ILE:HG12	2.55	0.41
1:A:291:ILE:HD11	1:A:698:PHE:CD2	2.54	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:478:LYS:HG3	1:A:479:GLN:N	2.35	0.41
1:A:654:ASN:HA	1:A:655:PRO:HD3	1.83	0.41
1:A:376:ASN:ND2	1:A:378:ASN:HD22	2.08	0.41
1:A:419:HIS:ND1	1:A:733:LEU:CD1	2.83	0.41
1:A:332:GLN:NE2	1:A:649:THR:OG1	2.34	0.41
1:A:247:ASN:N	1:A:247:ASN:ND2	2.69	0.41
1:A:436:TRP:CE2	1:A:458:LYS:HB2	2.55	0.41
1:A:438:LEU:HD12	1:A:438:LEU:C	2.41	0.41
1:A:254:LEU:HD11	1:A:267:SER:HB3	2.03	0.41
1:A:533:SER:OG	1:A:534:ASN:N	2.53	0.41
1:A:268:THR:HA	1:A:269:PRO:HD3	1.85	0.41
1:A:596:MET:HE2	1:A:597:GLY:N	2.35	0.41
1:A:334:PHE:HE1	1:A:645:PHE:HB2	1.81	0.41
1:A:678:VAL:O	1:A:678:VAL:HG12	2.21	0.41
1:A:720:GLU:HA	1:A:721:PRO:HD3	1.73	0.41
1:A:326:ASN:CG	1:A:329:SER:HB2	2.41	0.41
1:A:476:CYS:SG	1:A:477:VAL:N	2.86	0.41
1:A:363:VAL:HA	1:A:364:PRO:HD3	1.86	0.40
1:A:254:LEU:HA	1:A:254:LEU:HD22	1.67	0.40
1:A:257:THR:HA	1:A:262:THR:HB	2.03	0.40
1:A:372:VAL:CG1	1:A:512:ARG:HE	2.34	0.40
1:A:696:VAL:CG2	1:A:728:TYR:O	2.69	0.40
1:A:713:ASP:OD1	1:A:714:THR:N	2.55	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	518/733 (71%)	483 (93%)	33 (6%)	2 (0%)	43 90

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	655	PRO
1	A	652	PRO

### 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	447/609 (73%)	370 (83%)	77 (17%)	3 18

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	222	TRP
1	A	230	GLU
1	A	240	THR
1	A	250	LEU
1	A	254	LEU
1	A	257	THR
1	A	262	THR
1	A	263	TYR
1	A	274	ASP
1	A	275	PHE
1	A	277	ARG
1	A	279	HIS
1	A	297	LEU
1	A	303	ARG
1	A	308	ASN
1	A	318	ASN
1	A	320	GLU
1	A	326	ASN
1	A	329	SER
1	A	331	VAL
1	A	334	PHE
1	A	336	ASP
1	A	337	SER
1	A	338	SER
1	A	341	LEU
1	A	346	ASP

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Mol	Chain	Res	Type
1	A	352	SER
1	A	377	GLN
1	A	385	PHE
1	A	389	GLU
1	A	406	TYR
1	A	411	VAL
1	A	427	MET
1	A	432	ASP
1	A	438	LEU
1	A	439	GLN
1	A	440	SER
1	A	442	THR
1	A	445	GLU
1	A	469	LYS
1	A	472	LEU
1	A	475	PRO
1	A	476	CYS
1	A	481	ARG
1	A	504	ASP
1	A	507	TYR
1	A	509	LEU
1	A	512	ARG
1	A	515	ASN
1	A	516	ILE
1	A	544	VAL
1	A	548	THR
1	A	559	SER
1	A	561	GLU
1	A	566	THR
1	A	567	ASN
1	A	569	ARG
1	A	573	MET
1	A	592	ASN
1	A	594	THR
1	A	605	GLN
1	A	612	GLN
1	A	625	HIS
1	A	629	SER
1	A	631	LEU
1	A	638	LYS
1	A	647	LYS
1	A	648	ASN

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Mol	Chain	Res	Type
1	A	660	THR
1	A	663	ARG
1	A	675	GLN
1	A	678	VAL
1	A	698	PHE
1	A	699	THR
1	A	704	ASN
1	A	707	SER
1	A	715	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	279	HIS
1	A	288	GLN
1	A	292	ASN
1	A	294	ASN
1	A	308	ASN
1	A	365	GLN
1	A	377	GLN
1	A	378	ASN
1	A	383	ASN
1	A	400	ASN
1	A	407	ASN
1	A	480	GLN
1	A	510	ASN
1	A	536	GLN
1	A	583	ASN
1	A	605	GLN
1	A	606	ASN
1	A	627	HIS
1	A	643	GLN
1	A	648	ASN
1	A	697	GLN
1	A	704	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 ⓘ

There are no carbohydrates 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	801	-	24,24,24	0.64	0	36,36,36	1.04	3 (8%)

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	801	-	-	0/8/22/22	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	D5M	O2P-P-O1P	2.80	119.52	110.36
2	A	801	D5M	O3P-P-O5'	-2.43	99.70	106.67
2	A	801	D5M	C8-N9-C1'	2.31	130.51	126.15

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, 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	520/733 (70%)	-0.19	0 100 100	21, 41, 58, 92	0

There are no RSRZ outliers to report.

### 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 ⓘ

There are no carbohydrates in this entry.

### 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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	D5M	A	801	22/22	0.25	1.66	40,50,73,73	22

### 6.5 Other polymers ⓘ

There are no such residues in this entry.