



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 03:53 am BST

PDB ID : 1LP3  
Title : The Atomic Structure of Adeno-Associated Virus (AAV-2), a Vector for Human Gene Therapy  
Authors : Xie, Q.; Bu, W.; Bhatia, S.; Hare, J.; Somasundaram, T.; Azzi, A.; Chapman, M.S.  
Deposited on : 2002-05-07  
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.

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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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

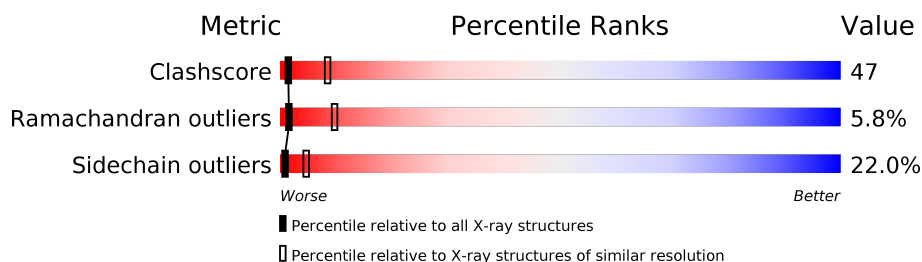
# 1 Overall quality at a glance

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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (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 on 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	519	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4152 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 AAV-2 capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	519	4152	2612	725	802	13	0	0	0



- Molecule 1: AAV-2 capsid protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	249.69Å 249.69Å 644.76Å 90.00° 101.16° 120.00°	Depositor
Resolution (Å)	39.80 – 3.00 98.69 – 3.03	Depositor EDS
% Data completeness (in resolution range)	56.0 (39.80-3.00) 57.2 (98.69-3.03)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.338 , 0.342 0.329 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.3	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , -6.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	0.499 for k,-h-k,h+l 0.499 for -h-k,h,h+k+l 0.115 for h,-h-k,-h-l 0.115 for k,h,-h-k-l 0.115 for -h-k,k,-l	Xtriage
$F_o, F_c$ correlation	0.73	EDS
Total number of atoms	4152	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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

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	0.94	3/4275 (0.1%)	1.06	7/5827 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	469	TRP	CB-CG	-5.94	1.39	1.50
1	A	563	TYR	CD2-CE2	5.48	1.47	1.39
1	A	346	TYR	CD1-CE1	5.29	1.47	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	496	LEU	CA-CB-CG	-8.49	95.77	115.30
1	A	205	VAL	CB-CA-C	-5.96	100.08	111.40
1	A	474	VAL	N-CA-C	5.77	126.57	111.00
1	A	510	LEU	CA-CB-CG	-5.76	102.05	115.30
1	A	353	LYS	CD-CE-NZ	5.25	123.78	111.70
1	A	382	PRO	CA-N-CD	-5.08	104.39	111.50
1	A	402	VAL	CB-CA-C	-5.05	101.81	111.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	276	TYR	Sidechain
1	A	475	TYR	Sidechain
1	A	593	TYR	Sidechain

## 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	4152	0	3904	378	0
All	All	4152	0	3904	378	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 47.

All (378) 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:347:ARG:NH1	1:A:438:GLN:H	1.56	1.03
1:A:372:HIS:HB3	1:A:377:ASP:OD1	1.64	0.98
1:A:204:GLN:HE22	1:A:514:THR:HG23	1.29	0.96
1:A:376:ARG:HG2	1:A:376:ARG:HH11	1.28	0.96
1:A:198:ASN:ND2	1:A:201:SER:HB2	1.83	0.94
1:A:552:GLU:HG2	1:A:553:ASN:H	1.31	0.94
1:A:266:LEU:HD23	1:A:270:ASN:HB3	1.54	0.89
1:A:445:ASN:H	1:A:454:ALA:HB3	1.37	0.88
1:A:179:PHE:HD1	1:A:180:ASN:HD22	1.18	0.87
1:A:472:ARG:HH11	1:A:472:ARG:HB3	1.40	0.87
1:A:174:LEU:HD12	1:A:174:LEU:C	1.96	0.86
1:A:389:HIS:NE2	1:A:426:GLU:OE1	2.09	0.86
1:A:295:ARG:HA	1:A:297:MET:HE1	1.57	0.86
1:A:381:ASN:CB	1:A:382:PRO:HD2	2.06	0.86
1:A:472:ARG:HD3	1:A:496:LEU:O	1.75	0.85
1:A:370:LYS:HA	1:A:380:VAL:HG23	1.58	0.85
1:A:103:ILE:N	1:A:103:ILE:HD12	1.92	0.85
1:A:574:ASP:HB3	1:A:586:PRO:HG2	1.57	0.85
1:A:228:PHE:CE2	1:A:230:ALA:HB3	2.13	0.84
1:A:182:GLN:HG3	1:A:538:THR:HG23	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:THR:CG2	1:A:565:SER:N	2.40	0.83
1:A:347:ARG:HH11	1:A:438:GLN:H	1.27	0.83
1:A:426:GLU:O	1:A:429:ARG:HG3	1.79	0.83
1:A:198:ASN:HD21	1:A:201:SER:HB2	1.43	0.82
1:A:312:ASN:HD22	1:A:312:ASN:C	1.78	0.82
1:A:389:HIS:CE1	1:A:424:ASP:OD2	2.32	0.82
1:A:381:ASN:CG	1:A:382:PRO:HD2	2.01	0.82
1:A:564:THR:HG22	1:A:565:SER:N	1.95	0.81
1:A:108:ARG:HH11	1:A:108:ARG:HG3	1.44	0.80
1:A:371:TYR:CD1	1:A:371:TYR:C	2.55	0.80
1:A:242:THR:HG21	1:A:254:SER:H	1.46	0.80
1:A:472:ARG:NH1	1:A:472:ARG:HB3	1.97	0.80
1:A:552:GLU:HG2	1:A:553:ASN:N	1.97	0.80
1:A:376:ARG:HG2	1:A:376:ARG:NH1	1.90	0.80
1:A:198:ASN:ND2	1:A:201:SER:CB	2.46	0.79
1:A:371:TYR:C	1:A:371:TYR:HD1	1.87	0.78
1:A:347:ARG:HH11	1:A:438:GLN:N	1.81	0.78
1:A:149:ARG:HD2	1:A:224:CYS:SG	2.23	0.78
1:A:108:ARG:HH11	1:A:108:ARG:CG	1.96	0.77
1:A:576:THR:HG22	1:A:577:VAL:N	1.99	0.77
1:A:394:GLU:OE1	1:A:426:GLU:OE1	2.03	0.77
1:A:483:LYS:HB2	1:A:505:PRO:HG2	1.66	0.77
1:A:289:HIS:HB2	1:A:430:THR:HG21	1.68	0.76
1:A:296:LEU:H	1:A:297:MET:HE3	1.50	0.76
1:A:347:ARG:NH1	1:A:438:GLN:N	2.33	0.76
1:A:385:ALA:HB2	1:A:472:ARG:HG2	1.66	0.76
1:A:362:GLU:OE1	1:A:362:GLU:HA	1.85	0.75
1:A:297:MET:HG2	1:A:336:GLN:OE1	1.86	0.75
1:A:204:GLN:NE2	1:A:514:THR:HG23	2.02	0.75
1:A:428:ILE:O	1:A:430:THR:N	2.20	0.74
1:A:384:PRO:HA	1:A:496:LEU:HD21	1.68	0.73
1:A:333:ILE:HG22	1:A:334:ARG:N	2.02	0.73
1:A:376:ARG:CG	1:A:376:ARG:HH11	2.01	0.72
1:A:472:ARG:CD	1:A:496:LEU:O	2.38	0.72
1:A:155:SER:O	1:A:156:PRO:C	2.27	0.71
1:A:381:ASN:HB3	1:A:382:PRO:HD2	1.71	0.70
1:A:242:THR:HG21	1:A:254:SER:N	2.06	0.70
1:A:372:HIS:HB2	1:A:377:ASP:HA	1.73	0.70
1:A:150:PHE:HB2	1:A:476:LEU:O	1.91	0.70
1:A:576:THR:CG2	1:A:577:VAL:N	2.55	0.69
1:A:186:VAL:HG13	1:A:534:THR:HG22	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:PHE:C	1:A:274:PHE:CD2	2.65	0.69
1:A:242:THR:HB	1:A:253:SER:HB2	1.75	0.69
1:A:424:ASP:OD2	1:A:426:GLU:OE1	2.10	0.69
1:A:329:GLY:H	1:A:332:ASP:HB2	1.57	0.69
1:A:562:GLN:HA	1:A:562:GLN:HE21	1.58	0.68
1:A:315:SER:HB3	1:A:318:THR:O	1.94	0.68
1:A:202:THR:HG22	1:A:267:ARG:HA	1.75	0.67
1:A:110:TRP:HB3	1:A:233:PHE:CE2	2.29	0.67
1:A:174:LEU:HG	1:A:276:TYR:HB3	1.75	0.67
1:A:295:ARG:HA	1:A:297:MET:CE	2.23	0.67
1:A:389:HIS:CE1	1:A:394:GLU:HA	2.30	0.67
1:A:394:GLU:OE2	1:A:424:ASP:OD2	2.14	0.66
1:A:510:LEU:HD12	1:A:510:LEU:N	2.11	0.66
1:A:215:TYR:CZ	1:A:217:LEU:HD12	2.31	0.65
1:A:174:LEU:CD1	1:A:174:LEU:C	2.65	0.65
1:A:284:HIS:NE2	1:A:591:THR:HG21	2.11	0.65
1:A:574:ASP:CB	1:A:586:PRO:HG2	2.27	0.65
1:A:312:ASN:HA	1:A:321:SER:HA	1.78	0.65
1:A:394:GLU:OE2	1:A:424:ASP:CG	2.35	0.65
1:A:312:ASN:ND2	1:A:312:ASN:C	2.50	0.65
1:A:473:ASP:OD1	1:A:591:THR:HG22	1.97	0.64
1:A:268:THR:HG22	1:A:269:GLY:N	2.12	0.64
1:A:184:LYS:HE2	1:A:197:ASN:CG	2.18	0.64
1:A:340:TRP:C	1:A:341:LEU:HD12	2.17	0.64
1:A:513:ASN:N	1:A:513:ASN:HD22	1.96	0.64
1:A:372:HIS:CB	1:A:377:ASP:HA	2.28	0.64
1:A:393:GLU:HB3	1:A:396:PHE:HD1	1.62	0.64
1:A:428:ILE:HG21	1:A:432:ASN:HB2	1.78	0.64
1:A:179:PHE:HD1	1:A:180:ASN:ND2	1.94	0.64
1:A:185:GLU:OE1	1:A:198:ASN:HB2	1.97	0.64
1:A:184:LYS:O	1:A:535:GLN:HB2	1.98	0.64
1:A:394:GLU:OE1	1:A:426:GLU:CD	2.36	0.64
1:A:398:PRO:HB2	1:A:401:GLY:H	1.62	0.64
1:A:165:ASN:HA	1:A:594:LEU:HD11	1.80	0.64
1:A:144:TYR:O	1:A:235:VAL:HG13	1.98	0.63
1:A:123:ILE:HG12	1:A:137:GLY:O	1.98	0.63
1:A:595:THR:HG22	1:A:595:THR:O	1.99	0.63
1:A:146:ASP:OD2	1:A:146:ASP:C	2.36	0.63
1:A:389:HIS:HE1	1:A:424:ASP:OD2	1.81	0.63
1:A:394:GLU:OE1	1:A:426:GLU:OE2	2.17	0.62
1:A:108:ARG:HD2	1:A:226:PRO:HD2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:ASP:O	1:A:575:PHE:HB2	2.00	0.62
1:A:389:HIS:NE2	1:A:394:GLU:OE1	2.32	0.62
1:A:281:VAL:HG22	1:A:282:PRO:CD	2.29	0.61
1:A:268:THR:HG22	1:A:269:GLY:H	1.66	0.61
1:A:354:THR:O	1:A:354:THR:HG22	2.01	0.61
1:A:284:HIS:CD2	1:A:591:THR:HG21	2.36	0.61
1:A:513:ASN:N	1:A:513:ASN:ND2	2.49	0.60
1:A:205:VAL:HG12	1:A:206:PHE:N	2.14	0.60
1:A:274:PHE:HD2	1:A:275:SER:N	1.99	0.60
1:A:222:GLN:O	1:A:222:GLN:HG3	2.01	0.60
1:A:363:TYR:N	1:A:363:TYR:CD1	2.69	0.60
1:A:381:ASN:CB	1:A:382:PRO:CD	2.80	0.60
1:A:157:ARG:NH1	1:A:161:ARG:HG2	2.16	0.60
1:A:267:ARG:H	1:A:270:ASN:HD22	1.48	0.60
1:A:228:PHE:HD2	1:A:231:ASP:OD1	1.85	0.59
1:A:341:LEU:CD1	1:A:341:LEU:N	2.65	0.59
1:A:394:GLU:CD	1:A:426:GLU:OE1	2.40	0.59
1:A:333:ILE:HA	1:A:336:GLN:HG3	1.83	0.59
1:A:444:THR:HB	1:A:454:ALA:HB1	1.85	0.59
1:A:126:GLN:HE21	1:A:126:GLN:CA	2.16	0.58
1:A:152:CYS:SG	1:A:225:LEU:HB2	2.43	0.58
1:A:475:TYR:HA	1:A:589:ILE:O	2.03	0.58
1:A:325:PHE:N	1:A:325:PHE:CD2	2.72	0.58
1:A:120:TYR:OH	1:A:258:LEU:HB2	2.04	0.58
1:A:312:ASN:HB2	1:A:319:THR:OG1	2.04	0.58
1:A:381:ASN:HB3	1:A:382:PRO:CD	2.34	0.58
1:A:472:ARG:HH11	1:A:472:ARG:CB	2.14	0.58
1:A:461:GLN:HA	1:A:461:GLN:OE1	2.03	0.58
1:A:428:ILE:CG2	1:A:432:ASN:HB2	2.34	0.57
1:A:444:THR:HB	1:A:454:ALA:CB	2.34	0.57
1:A:174:LEU:HD12	1:A:175:ASN:N	2.19	0.57
1:A:371:TYR:O	1:A:371:TYR:HD1	1.87	0.57
1:A:410:SER:OG	1:A:419:LYS:HB3	2.04	0.57
1:A:370:LYS:HB2	1:A:378:SER:O	2.04	0.57
1:A:371:TYR:O	1:A:371:TYR:CD1	2.58	0.57
1:A:184:LYS:HE2	1:A:197:ASN:OD1	2.04	0.57
1:A:186:VAL:CG1	1:A:534:THR:HG22	2.34	0.57
1:A:284:HIS:NE2	1:A:474:VAL:HG22	2.19	0.57
1:A:470:GLN:CA	1:A:470:GLN:HE21	2.18	0.56
1:A:281:VAL:HG22	1:A:282:PRO:HD2	1.87	0.56
1:A:296:LEU:O	1:A:296:LEU:HD23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LEU:HD11	1:A:510:LEU:HD22	1.86	0.56
1:A:215:TYR:HA	1:A:508:GLN:OE1	2.05	0.56
1:A:160:GLN:O	1:A:163:ILE:HG22	2.05	0.56
1:A:276:TYR:CD2	1:A:277:THR:N	2.73	0.56
1:A:274:PHE:CD2	1:A:275:SER:N	2.74	0.56
1:A:394:GLU:OE2	1:A:426:GLU:OE1	2.23	0.56
1:A:596:ARG:HG2	1:A:597:ASN:N	2.21	0.56
1:A:205:VAL:HG23	1:A:266:LEU:HD12	1.88	0.56
1:A:188:GLN:HG2	1:A:193:THR:HG22	1.86	0.56
1:A:208:ASP:O	1:A:208:ASP:CG	2.43	0.56
1:A:176:PHE:CD2	1:A:177:LYS:N	2.74	0.55
1:A:228:PHE:HE2	1:A:230:ALA:HB3	1.66	0.55
1:A:384:PRO:O	1:A:386:MET:HG2	2.06	0.55
1:A:464:LEU:O	1:A:467:MET:HG3	2.05	0.55
1:A:577:VAL:HB	1:A:581:GLY:HA2	1.87	0.55
1:A:165:ASN:C	1:A:166:ASN:ND2	2.59	0.55
1:A:392:ASP:C	1:A:393:GLU:HG2	2.25	0.55
1:A:167:TRP:HA	1:A:167:TRP:HE3	1.70	0.55
1:A:242:THR:HG21	1:A:253:SER:HA	1.88	0.55
1:A:103:ILE:N	1:A:103:ILE:CD1	2.63	0.55
1:A:333:ILE:O	1:A:334:ARG:C	2.45	0.55
1:A:438:GLN:HB2	1:A:458:VAL:O	2.07	0.55
1:A:108:ARG:NH1	1:A:108:ARG:HG3	2.16	0.55
1:A:412:LYS:HG2	1:A:412:LYS:O	2.07	0.55
1:A:343:GLY:O	1:A:439:TYR:HE1	1.89	0.54
1:A:287:TYR:CD1	1:A:596:ARG:HB3	2.43	0.54
1:A:148:ASN:ND2	1:A:481:TRP:CE2	2.76	0.54
1:A:389:HIS:CE1	1:A:426:GLU:OE1	2.61	0.54
1:A:117:ASN:O	1:A:118:HIS:HB2	2.08	0.54
1:A:381:ASN:O	1:A:382:PRO:C	2.43	0.54
1:A:186:VAL:HG13	1:A:534:THR:CG2	2.38	0.54
1:A:126:GLN:O	1:A:128:GLY:N	2.41	0.54
1:A:202:THR:HG22	1:A:267:ARG:CA	2.37	0.54
1:A:344:PRO:HB3	1:A:467:MET:HE1	1.90	0.54
1:A:513:ASN:HD22	1:A:513:ASN:H	1.54	0.54
1:A:170:ARG:HD2	1:A:281:VAL:HG12	1.90	0.54
1:A:132:ASP:HA	1:A:376:ARG:HB3	1.90	0.53
1:A:176:PHE:C	1:A:176:PHE:CD2	2.81	0.53
1:A:167:TRP:HA	1:A:167:TRP:CE3	2.43	0.53
1:A:202:THR:HG22	1:A:266:LEU:O	2.08	0.53
1:A:354:THR:HB	1:A:357:ASP:OD2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:LEU:CD1	1:A:175:ASN:N	2.71	0.53
1:A:381:ASN:OD1	1:A:382:PRO:HD2	2.07	0.53
1:A:242:THR:CG2	1:A:253:SER:HA	2.39	0.53
1:A:553:ASN:CG	1:A:553:ASN:O	2.47	0.53
1:A:389:HIS:CE1	1:A:394:GLU:CD	2.82	0.53
1:A:122:GLN:NE2	1:A:136:PHE:CE1	2.77	0.52
1:A:301:ILE:HG22	1:A:302:ASP:O	2.09	0.52
1:A:304:TYR:CD2	1:A:305:LEU:HD13	2.44	0.52
1:A:552:GLU:O	1:A:553:ASN:HB2	2.08	0.52
1:A:170:ARG:HB2	1:A:171:PRO:HD2	1.91	0.52
1:A:393:GLU:HB3	1:A:396:PHE:CD1	2.43	0.52
1:A:287:TYR:O	1:A:592:ARG:HG2	2.10	0.52
1:A:286:SER:HA	1:A:591:THR:CG2	2.40	0.52
1:A:341:LEU:HD12	1:A:341:LEU:N	2.24	0.52
1:A:564:THR:HG23	1:A:565:SER:H	1.75	0.52
1:A:564:THR:CG2	1:A:565:SER:H	2.23	0.52
1:A:146:ASP:O	1:A:224:CYS:HA	2.10	0.51
1:A:206:PHE:C	1:A:206:PHE:CD1	2.84	0.51
1:A:188:GLN:CG	1:A:193:THR:HG22	2.40	0.51
1:A:296:LEU:H	1:A:297:MET:CE	2.22	0.51
1:A:155:SER:O	1:A:158:ASP:N	2.44	0.51
1:A:283:PHE:CD1	1:A:550:GLN:HB2	2.45	0.51
1:A:371:TYR:CE1	1:A:378:SER:HB2	2.46	0.51
1:A:215:TYR:OH	1:A:505:PRO:HB2	2.10	0.51
1:A:126:GLN:HE21	1:A:126:GLN:HA	1.75	0.51
1:A:450:ASN:H	1:A:450:ASN:ND2	2.07	0.51
1:A:556:ARG:HH21	1:A:558:ASN:HD21	1.59	0.51
1:A:595:THR:CG2	1:A:595:THR:O	2.59	0.51
1:A:242:THR:CB	1:A:253:SER:HB2	2.42	0.50
1:A:576:THR:CG2	1:A:577:VAL:H	2.23	0.50
1:A:347:ARG:HD3	1:A:459:ASN:OD1	2.11	0.50
1:A:428:ILE:O	1:A:429:ARG:C	2.49	0.50
1:A:189:ASN:O	1:A:192:THR:HG23	2.11	0.50
1:A:125:SER:CB	1:A:134:HIS:HA	2.40	0.50
1:A:157:ARG:HH12	1:A:161:ARG:HG2	1.76	0.50
1:A:174:LEU:HD12	1:A:174:LEU:O	2.11	0.50
1:A:294:ASP:O	1:A:297:MET:HE3	2.11	0.50
1:A:548:GLU:HG2	1:A:549:LEU:N	2.27	0.50
1:A:242:THR:HG21	1:A:253:SER:CA	2.41	0.49
1:A:564:THR:HG22	1:A:565:SER:O	2.12	0.49
1:A:165:ASN:C	1:A:166:ASN:HD22	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:PHE:CD1	1:A:532:PHE:N	2.80	0.49
1:A:267:ARG:O	1:A:270:ASN:HB2	2.12	0.49
1:A:144:TYR:CE2	1:A:236:PRO:HB2	2.47	0.49
1:A:286:SER:CB	1:A:591:THR:HG23	2.43	0.49
1:A:208:ASP:O	1:A:210:GLU:N	2.46	0.49
1:A:242:THR:HG22	1:A:243:LEU:HD12	1.93	0.49
1:A:328:ALA:HB1	1:A:336:GLN:HG2	1.93	0.49
1:A:198:ASN:ND2	1:A:201:SER:HB3	2.27	0.49
1:A:513:ASN:O	1:A:514:THR:C	2.51	0.49
1:A:574:ASP:O	1:A:575:PHE:CB	2.61	0.49
1:A:172:LYS:HB2	1:A:546:GLU:HG2	1.95	0.48
1:A:516:VAL:HG12	1:A:533:ILE:HG13	1.94	0.48
1:A:187:THR:O	1:A:193:THR:HA	2.14	0.48
1:A:206:PHE:HB3	1:A:263:SER:HA	1.96	0.48
1:A:283:PHE:CE1	1:A:550:GLN:HB2	2.49	0.48
1:A:198:ASN:HD22	1:A:201:SER:CB	2.27	0.47
1:A:398:PRO:HB2	1:A:401:GLY:N	2.29	0.47
1:A:200:THR:O	1:A:201:SER:C	2.53	0.47
1:A:372:HIS:CB	1:A:377:ASP:OD1	2.50	0.47
1:A:84:VAL:HG12	1:A:85:GLY:N	2.29	0.47
1:A:149:ARG:HD2	1:A:224:CYS:HB2	1.97	0.47
1:A:538:THR:OG1	1:A:539:GLY:N	2.47	0.47
1:A:126:GLN:NE2	1:A:126:GLN:HA	2.30	0.47
1:A:445:ASN:C	1:A:445:ASN:OD1	2.53	0.47
1:A:481:TRP:CD1	1:A:482:ALA:N	2.83	0.47
1:A:158:ASP:HA	1:A:161:ARG:HG3	1.97	0.47
1:A:407:LYS:O	1:A:408:GLN:C	2.53	0.47
1:A:518:ALA:H	1:A:532:PHE:HA	1.80	0.47
1:A:470:GLN:CA	1:A:470:GLN:NE2	2.78	0.47
1:A:474:VAL:O	1:A:475:TYR:HB2	2.15	0.47
1:A:349:GLN:CB	1:A:399:GLN:OE1	2.63	0.46
1:A:125:SER:HB3	1:A:135:TYR:N	2.31	0.46
1:A:575:PHE:CZ	1:A:586:PRO:HD2	2.50	0.46
1:A:163:ILE:HD11	1:A:591:THR:HA	1.97	0.46
1:A:128:GLY:O	1:A:129:ALA:O	2.33	0.46
1:A:473:ASP:OD1	1:A:591:THR:CG2	2.64	0.46
1:A:103:ILE:HD12	1:A:103:ILE:H	1.75	0.46
1:A:473:ASP:OD2	1:A:591:THR:N	2.46	0.46
1:A:243:LEU:HD13	1:A:253:SER:N	2.31	0.46
1:A:258:LEU:CD1	1:A:510:LEU:HD22	2.46	0.46
1:A:149:ARG:HD2	1:A:224:CYS:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:GLU:O	1:A:185:GLU:HG3	2.17	0.45
1:A:360:ASN:O	1:A:361:SER:HB3	2.16	0.45
1:A:243:LEU:HD12	1:A:253:SER:HA	1.98	0.45
1:A:156:PRO:O	1:A:157:ARG:C	2.54	0.45
1:A:189:ASN:O	1:A:192:THR:CG2	2.64	0.45
1:A:125:SER:OG	1:A:134:HIS:ND1	2.30	0.45
1:A:122:GLN:NE2	1:A:136:PHE:HE1	2.13	0.45
1:A:170:ARG:HB3	1:A:283:PHE:HD2	1.82	0.45
1:A:428:ILE:HG21	1:A:432:ASN:CB	2.47	0.45
1:A:144:TYR:O	1:A:236:PRO:HD2	2.16	0.45
1:A:349:GLN:HA	1:A:349:GLN:OE1	2.16	0.45
1:A:206:PHE:CB	1:A:263:SER:HA	2.47	0.45
1:A:313:THR:HB	1:A:322:ARG:HB3	1.98	0.45
1:A:395:LYS:HE2	1:A:396:PHE:CZ	2.52	0.45
1:A:438:GLN:HG3	1:A:457:ASP:HB3	1.99	0.45
1:A:511:ILE:HG23	1:A:511:ILE:O	2.17	0.45
1:A:279:GLU:OE2	1:A:503:LYS:HB3	2.17	0.44
1:A:417:ILE:HG23	1:A:418:GLU:N	2.32	0.44
1:A:178:LEU:HD23	1:A:541:VAL:HG23	1.98	0.44
1:A:545:ILE:HG22	1:A:546:GLU:N	2.31	0.44
1:A:217:LEU:HG	1:A:217:LEU:H	1.40	0.44
1:A:386:MET:SD	1:A:435:ALA:HA	2.58	0.44
1:A:350:ARG:HB2	1:A:436:THR:HG21	1.99	0.44
1:A:458:VAL:HG22	1:A:458:VAL:O	2.17	0.44
1:A:107:THR:HG23	1:A:541:VAL:O	2.17	0.44
1:A:148:ASN:ND2	1:A:481:TRP:CD2	2.85	0.44
1:A:260:TYR:O	1:A:260:TYR:HD1	2.01	0.44
1:A:470:GLN:NE2	1:A:470:GLN:HA	2.32	0.44
1:A:545:ILE:CG2	1:A:546:GLU:N	2.79	0.44
1:A:190:ASP:HB2	1:A:191:GLY:H	1.57	0.44
1:A:432:ASN:N	1:A:432:ASN:OD1	2.49	0.44
1:A:385:ALA:CB	1:A:472:ARG:HG2	2.43	0.44
1:A:220:ALA:HB2	1:A:497:MET:SD	2.58	0.44
1:A:187:THR:HG22	1:A:189:ASN:ND2	2.33	0.44
1:A:315:SER:CB	1:A:318:THR:O	2.65	0.44
1:A:200:THR:O	1:A:201:SER:O	2.35	0.44
1:A:552:GLU:CG	1:A:553:ASN:N	2.73	0.44
1:A:182:GLN:HG3	1:A:538:THR:CG2	2.40	0.43
1:A:116:ASN:HB3	1:A:119:LEU:O	2.18	0.43
1:A:158:ASP:O	1:A:159:TRP:C	2.56	0.43
1:A:512:LYS:HG2	1:A:513:ASN:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:SER:HA	1:A:430:THR:OG1	2.18	0.43
1:A:360:ASN:O	1:A:361:SER:CB	2.65	0.43
1:A:388:SER:O	1:A:389:HIS:HB3	2.18	0.43
1:A:102:VAL:HG13	1:A:102:VAL:O	2.18	0.43
1:A:360:ASN:OD1	1:A:360:ASN:C	2.57	0.43
1:A:243:LEU:HB2	1:A:253:SER:HB3	2.01	0.43
1:A:519:ASN:HA	1:A:520:PRO:HD3	1.68	0.43
1:A:101:ARG:C	1:A:102:VAL:HG12	2.38	0.43
1:A:151:HIS:CE1	1:A:227:PRO:HG3	2.54	0.43
1:A:170:ARG:HG2	1:A:283:PHE:HE2	1.83	0.43
1:A:107:THR:HG23	1:A:542:SER:HB2	2.00	0.43
1:A:108:ARG:NH1	1:A:108:ARG:CG	2.66	0.43
1:A:123:ILE:O	1:A:123:ILE:CG1	2.65	0.43
1:A:293:LEU:HA	1:A:293:LEU:HD23	1.73	0.43
1:A:379:LEU:HD12	1:A:380:VAL:H	1.84	0.43
1:A:112:LEU:HA	1:A:113:PRO:HD3	1.65	0.42
1:A:120:TYR:OH	1:A:259:GLU:OE1	2.35	0.42
1:A:350:ARG:HD2	1:A:396:PHE:CG	2.54	0.42
1:A:397:PHE:HB2	1:A:398:PRO:CD	2.49	0.42
1:A:576:THR:HG22	1:A:577:VAL:O	2.19	0.42
1:A:181:ILE:O	1:A:268:THR:HG23	2.19	0.42
1:A:91:TRP:CD1	1:A:91:TRP:C	2.92	0.42
1:A:428:ILE:HD13	1:A:428:ILE:HG21	1.79	0.42
1:A:520:PRO:HB3	1:A:529:PHE:HZ	1.85	0.42
1:A:204:GLN:H	1:A:204:GLN:HG2	1.63	0.42
1:A:235:VAL:HA	1:A:236:PRO:HD3	1.82	0.42
1:A:342:PRO:HD2	1:A:439:TYR:OH	2.20	0.42
1:A:469:TRP:CD1	1:A:469:TRP:C	2.93	0.42
1:A:91:TRP:NE1	1:A:93:CYS:HB2	2.34	0.42
1:A:128:GLY:O	1:A:129:ALA:C	2.58	0.42
1:A:349:GLN:HB2	1:A:399:GLN:OE1	2.20	0.42
1:A:428:ILE:C	1:A:430:THR:N	2.74	0.42
1:A:175:ASN:HD22	1:A:176:PHE:N	2.17	0.42
1:A:242:THR:HB	1:A:253:SER:CB	2.47	0.42
1:A:305:LEU:HD12	1:A:305:LEU:HA	1.68	0.42
1:A:198:ASN:O	1:A:199:LEU:C	2.58	0.41
1:A:447:GLN:OE1	1:A:447:GLN:C	2.59	0.41
1:A:384:PRO:CA	1:A:496:LEU:HD21	2.44	0.41
1:A:110:TRP:CD1	1:A:539:GLY:O	2.73	0.41
1:A:179:PHE:O	1:A:180:ASN:HB2	2.20	0.41
1:A:160:GLN:HA	1:A:163:ILE:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:VAL:HG22	1:A:397:PHE:O	2.20	0.41
1:A:289:HIS:HA	1:A:596:ARG:O	2.20	0.41
1:A:163:ILE:CD1	1:A:591:THR:HA	2.51	0.41
1:A:174:LEU:HB2	1:A:545:ILE:HG12	2.03	0.41
1:A:347:ARG:NH1	1:A:438:GLN:HB3	2.35	0.41
1:A:564:THR:HG22	1:A:565:SER:C	2.41	0.41
1:A:109:THR:HB	1:A:232:VAL:HG22	2.03	0.41
1:A:279:GLU:O	1:A:280:ASP:C	2.58	0.41
1:A:298:ASN:HA	1:A:299:PRO:HD3	1.77	0.41
1:A:96:THR:O	1:A:102:VAL:HA	2.19	0.41
1:A:176:PHE:CE2	1:A:178:LEU:HG	2.55	0.41
1:A:415:VAL:HG22	1:A:419:LYS:CG	2.50	0.41
1:A:556:ARG:NH1	1:A:560:GLU:OE1	2.40	0.41
1:A:285:SER:HB2	1:A:287:TYR:CE2	2.55	0.41
1:A:163:ILE:HG13	1:A:591:THR:HA	2.02	0.41
1:A:349:GLN:HB3	1:A:399:GLN:OE1	2.21	0.41
1:A:215:TYR:CE1	1:A:217:LEU:HD12	2.55	0.41
1:A:276:TYR:CG	1:A:277:THR:N	2.89	0.41
1:A:294:ASP:O	1:A:297:MET:CE	2.69	0.41
1:A:341:LEU:O	1:A:467:MET:HA	2.21	0.41
1:A:563:TYR:C	1:A:563:TYR:CD2	2.93	0.41
1:A:389:HIS:NE2	1:A:394:GLU:CD	2.74	0.41
1:A:393:GLU:C	1:A:395:LYS:N	2.73	0.41
1:A:552:GLU:O	1:A:553:ASN:CB	2.66	0.41
1:A:92:HIS:HB3	1:A:105:THR:HG21	2.03	0.40
1:A:177:LYS:HA	1:A:272:PHE:O	2.21	0.40
1:A:122:GLN:HG2	1:A:123:ILE:N	2.36	0.40
1:A:175:ASN:HD22	1:A:176:PHE:H	1.68	0.40
1:A:177:LYS:HE2	1:A:179:PHE:CD2	2.57	0.40
1:A:167:TRP:HB3	1:A:550:GLN:HE21	1.87	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	517/519 (100%)	402 (78%)	85 (16%)	30 (6%)	1 10

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	SER
1	A	129	ALA
1	A	156	PRO
1	A	199	LEU
1	A	209	SER
1	A	333	ILE
1	A	356	ALA
1	A	382	PRO
1	A	429	ARG
1	A	553	ASN
1	A	82	ASP
1	A	192	THR
1	A	201	SER
1	A	217	LEU
1	A	473	ASP
1	A	519	ASN
1	A	578	ASP
1	A	102	VAL
1	A	223	GLY
1	A	347	ARG
1	A	361	SER
1	A	417	ILE
1	A	427	GLU
1	A	294	ASP
1	A	355	SER
1	A	387	ALA
1	A	230	ALA
1	A	475	TYR
1	A	214	PRO
1	A	262	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	459/459 (100%)	358 (78%)	101 (22%)	<b>1</b> <b>4</b>

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ASP
1	A	84	VAL
1	A	88	SER
1	A	96	THR
1	A	98	MET
1	A	102	VAL
1	A	106	SER
1	A	108	ARG
1	A	119	LEU
1	A	126	GLN
1	A	146	ASP
1	A	151	HIS
1	A	156	PRO
1	A	162	LEU
1	A	165	ASN
1	A	167	TRP
1	A	173	ARG
1	A	174	LEU
1	A	175	ASN
1	A	176	PHE
1	A	184	LYS
1	A	186	VAL
1	A	190	ASP
1	A	194	THR
1	A	203	VAL
1	A	206	PHE
1	A	207	THR
1	A	208	ASP
1	A	210	GLU
1	A	217	LEU
1	A	231	ASP
1	A	242	THR
1	A	257	CYS
1	A	258	LEU

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Mol	Chain	Res	Type
1	A	260	TYR
1	A	263	SER
1	A	264	GLN
1	A	273	THR
1	A	274	PHE
1	A	275	SER
1	A	290	SER
1	A	296	LEU
1	A	297	MET
1	A	302	ASP
1	A	305	LEU
1	A	308	LEU
1	A	309	SER
1	A	312	ASN
1	A	313	THR
1	A	317	THR
1	A	319	THR
1	A	320	GLN
1	A	323	LEU
1	A	332	ASP
1	A	339	ASN
1	A	341	LEU
1	A	345	CYS
1	A	349	GLN
1	A	352	SER
1	A	362	GLU
1	A	363	TYR
1	A	366	THR
1	A	369	THR
1	A	371	TYR
1	A	372	HIS
1	A	376	ARG
1	A	390	LYS
1	A	393	GLU
1	A	403	LEU
1	A	408	GLN
1	A	413	THR
1	A	415	VAL
1	A	416	ASP
1	A	417	ILE
1	A	418	GLU
1	A	424	ASP

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Mol	Chain	Res	Type
1	A	426	GLU
1	A	450	ASN
1	A	458	VAL
1	A	470	GLN
1	A	472	ARG
1	A	474	VAL
1	A	494	SER
1	A	496	LEU
1	A	507	PRO
1	A	508	GLN
1	A	513	ASN
1	A	514	THR
1	A	522	THR
1	A	529	PHE
1	A	531	SER
1	A	540	GLN
1	A	559	PRO
1	A	562	GLN
1	A	565	SER
1	A	566	ASN
1	A	568	ASN
1	A	579	THR
1	A	591	THR
1	A	595	THR
1	A	598	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	GLN
1	A	160	GLN
1	A	166	ASN
1	A	175	ASN
1	A	180	ASN
1	A	189	ASN
1	A	198	ASN
1	A	204	GLN
1	A	248	GLN
1	A	270	ASN
1	A	312	ASN
1	A	470	GLN
1	A	513	ASN

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Mol	Chain	Res	Type
1	A	535	GLN
1	A	558	ASN
1	A	562	GLN

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.