



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 07:20 PM GMT

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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

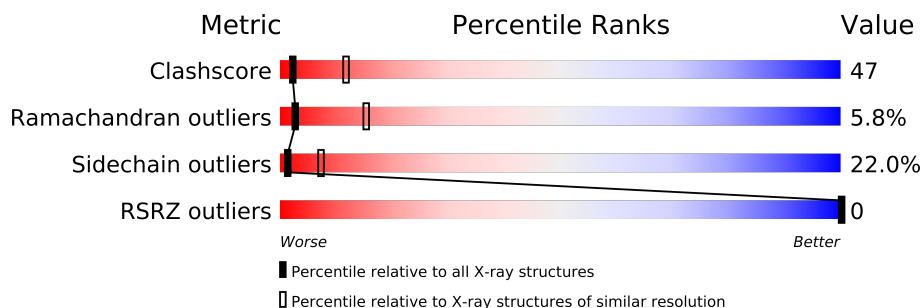
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
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) : stable22683

1 Overall quality at a glance

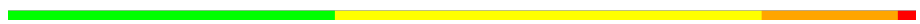
The reported resolution of this entry is 3.00 Å.

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	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (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 ≥ 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	519	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4152 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.

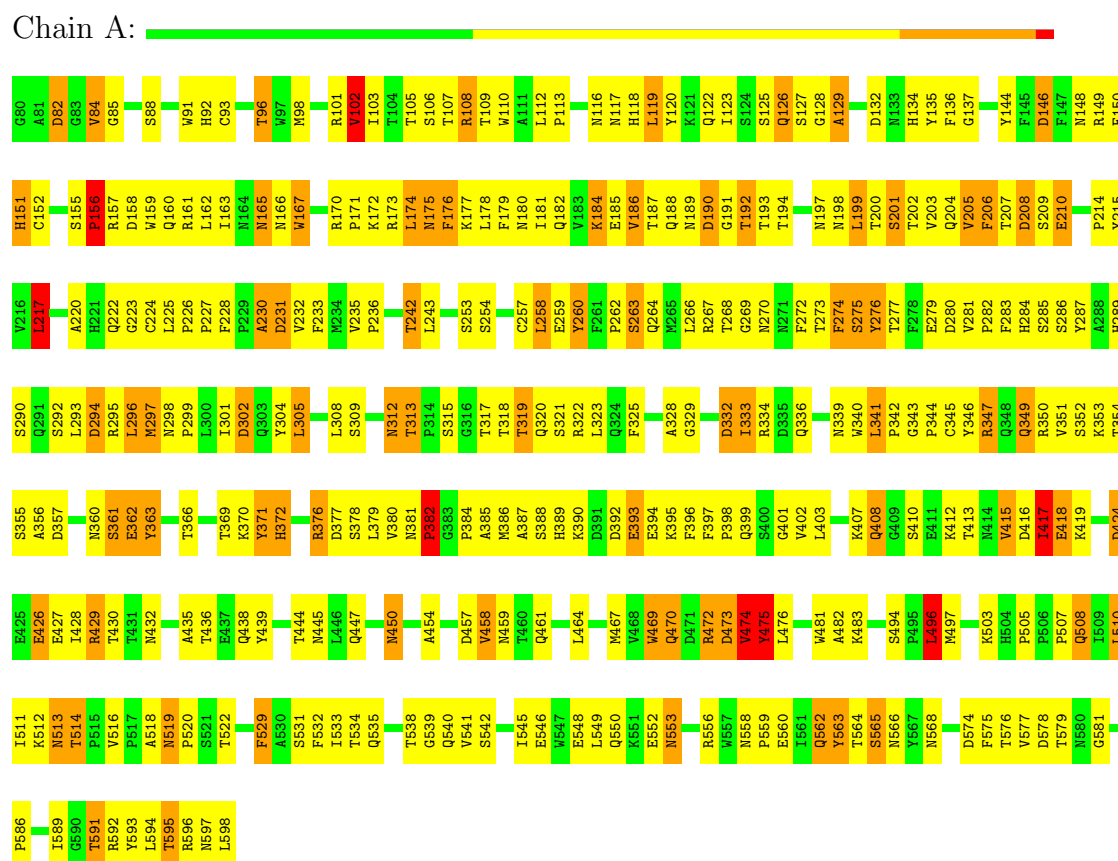
- Molecule 1 is a protein called AAV-2 capsid protein.

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

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: AAV-2 capsid protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.338 , 0.342 0.346 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	37.3	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , -8.9	EDS
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
L-test for twinning	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtriage
Outliers	0 of 2554728 reflections	Xtriage
F_o, F_c correlation	0.73	EDS
Total number of atoms	4152	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

All (378) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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:347:ARG:NH1	1:A:438:GLN:N	2.33	0.76
1:A:296:LEU:H	1:A:297:MET:HE3	1.50	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
1:A:274:PHE:C	1:A:274:PHE:CD2	2.65	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:424:ASP:OD2	1:A:426:GLU:OE1	2.10	0.69
1:A:242:THR:HB	1:A:253:SER:HB2	1.75	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:389:HIS:CE1	1:A:394:GLU:HA	2.30	0.67
1:A:295:ARG:HA	1:A:297:MET:CE	2.23	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:394:GLU:OE2	1:A:424:ASP:CG	2.35	0.65
1:A:312:ASN:HA	1:A:321:SER:HA	1.78	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:185:GLU:OE1	1:A:198:ASN:HB2	1.97	0.64
1:A:179:PHE:HD1	1:A:180:ASN:ND2	1.94	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:ND2	1:A:513:ASN:N	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:HG3	1:A:222:GLN:O	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:394:GLU:CD	1:A:426:GLU:OE1	2.40	0.59
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:444:THR:HB	1:A:454:ALA:HB1	1.85	0.59
1:A:333:ILE:HA	1:A:336:GLN:HG3	1.83	0.59
1:A:152:CYS:SG	1:A:225:LEU:HB2	2.43	0.58
1:A:126:GLN:HE21	1:A:126:GLN:CA	2.16	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:472:ARG:HH11	1:A:472:ARG:CB	2.14	0.58
1:A:381:ASN:HB3	1:A:382:PRO:CD	2.34	0.58
1:A:312:ASN:HB2	1:A:319:THR:OG1	2.04	0.58
1:A:120:TYR:OH	1:A:258:LEU:HB2	2.04	0.58
1:A:461:GLN:HA	1:A:461:GLN:OE1	2.03	0.58
1:A:444:THR:HB	1:A:454:ALA:CB	2.34	0.57
1:A:428:ILE:CG2	1:A:432:ASN:HB2	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:371:TYR:O	1:A:371:TYR:CD1	2.58	0.57
1:A:370:LYS:HB2	1:A:378:SER:O	2.04	0.57
1:A:186:VAL:CG1	1:A:534:THR:HG22	2.34	0.57
1:A:184:LYS:HE2	1:A:197:ASN:OD1	2.04	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:296:LEU:O	1:A:296:LEU:HD23	2.05	0.56
1:A:281:VAL:HG22	1:A:282:PRO:HD2	1.87	0.56
1:A:215:TYR:HA	1:A:508:GLN:OE1	2.05	0.56
1:A:258:LEU:HD11	1:A:510:LEU:HD22	1.86	0.56
1:A:276:TYR:CD2	1:A:277:THR:N	2.73	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:160:GLN:O	1:A:163:ILE:HG22	2.05	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:274:PHE:CD2	1:A:275:SER:N	2.74	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:CG	1:A:208:ASP:O	2.43	0.56
1:A:176:PHE:CD2	1:A:177:LYS:N	2.74	0.55
1:A:384:PRO:O	1:A:386:MET:HG2	2.06	0.55
1:A:228:PHE:HE2	1:A:230:ALA:HB3	1.66	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:392:ASP:C	1:A:393:GLU:HG2	2.25	0.55
1:A:165:ASN:C	1:A:166:ASN:ND2	2.59	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:333:ILE:O	1:A:334:ARG:C	2.45	0.55
1:A:103:ILE:N	1:A:103:ILE:CD1	2.63	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:381:ASN:O	1:A:382:PRO:C	2.43	0.54
1:A:117:ASN:O	1:A:118:HIS:HB2	2.08	0.54
1:A:186:VAL:HG13	1:A:534:THR:CG2	2.38	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:126:GLN:O	1:A:128:GLY:N	2.41	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:202:THR:HG22	1:A:266:LEU:O	2.08	0.53
1:A:167:TRP:HA	1:A:167:TRP:CE3	2.43	0.53
1:A:354:THR:HB	1:A:357:ASP:OD2	2.09	0.53
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:552:GLU:O	1:A:553:ASN:HB2	2.08	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:170:ARG:HB2	1:A:171:PRO:HD2	1.91	0.52
1:A:287:TYR:O	1:A:592:ARG:HG2	2.10	0.52
1:A:393:GLU:HB3	1:A:396:PHE:CD1	2.43	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:296:LEU:H	1:A:297:MET:CE	2.22	0.51
1:A:188:GLN:CG	1:A:193:THR:HG22	2.40	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: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:126:GLN:HE21	1:A:126:GLN:HA	1.75	0.51
1:A:556:ARG:HH21	1:A:558:ASN:HD21	1.59	0.51
1:A:450:ASN:H	1:A:450:ASN:ND2	2.07	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:157:ARG:HH12	1:A:161:ARG:HG2	1.76	0.50
1:A:125:SER:CB	1:A:134:HIS:HA	2.40	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:564:THR:HG22	1:A:565:SER:O	2.12	0.49
1:A:242:THR:HG21	1:A:253:SER:CA	2.41	0.49
1:A:165:ASN:C	1:A:166:ASN:HD22	2.16	0.49
1:A:532:PHE:N	1:A:532:PHE:CD1	2.80	0.49
1:A:267:ARG:O	1:A:270:ASN:HB2	2.12	0.49
1:A:286:SER:CB	1:A:591:THR:HG23	2.43	0.49
1:A:144:TYR:CE2	1:A:236:PRO:HB2	2.47	0.49
1:A:328:ALA:HB1	1:A:336:GLN:HG2	1.93	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:242:THR:HG22	1:A:243:LEU:HD12	1.93	0.49
1:A:208:ASP:O	1:A:210:GLU:N	2.46	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: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:187:THR:O	1:A:193:THR:HA	2.14	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:372:HIS:CB	1:A:377:ASP:OD1	2.50	0.47
1:A:200:THR:O	1:A:201:SER:C	2.53	0.47
1:A:84:VAL:HG12	1:A:85:GLY:N	2.29	0.47
1:A:538:THR:OG1	1:A:539:GLY:N	2.47	0.47
1:A:149:ARG:HD2	1:A:224:CYS:HB2	1.97	0.47
1:A:445:ASN:C	1:A:445:ASN:OD1	2.53	0.47
1:A:126:GLN:NE2	1:A:126:GLN:HA	2.30	0.47
1:A:158:ASP:HA	1:A:161:ARG:HG3	1.97	0.47
1:A:481:TRP:CD1	1:A:482:ALA:N	2.83	0.47
1:A:518:ALA:H	1:A:532:PHE:HA	1.80	0.47
1:A:407:LYS:O	1:A:408:GLN:C	2.53	0.47
1:A:470:GLN:NE2	1:A:470:GLN:CA	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:185:GLU:O	1:A:185:GLU:HG3	2.17	0.45
1:A:149:ARG:HD2	1:A:224:CYS:CB	2.47	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:122:GLN:NE2	1:A:136:PHE:HE1	2.13	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:170:ARG:HB3	1:A:283:PHE:HD2	1.82	0.45
1:A:125:SER:OG	1:A:134:HIS:ND1	2.30	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:438:GLN:HG3	1:A:457:ASP:HB3	1.99	0.45
1:A:395:LYS:HE2	1:A:396:PHE:CZ	2.52	0.45
1:A:511:ILE:HG23	1:A:511:ILE:O	2.17	0.45
1:A:417:ILE:HG23	1:A:418:GLU:N	2.32	0.44
1:A:279:GLU:OE2	1:A:503:LYS:HB3	2.17	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:458:VAL:HG22	1:A:458:VAL:O	2.17	0.44
1:A:386:MET:SD	1:A:435:ALA:HA	2.58	0.44
1:A:217:LEU:HG	1:A:217:LEU:H	1.40	0.44
1:A:350:ARG:HB2	1:A:436:THR:HG21	1.99	0.44
1:A:107:THR:HG23	1:A:541:VAL:O	2.17	0.44
1:A:545:ILE:CG2	1:A:546:GLU:N	2.79	0.44
1:A:470:GLN:NE2	1:A:470:GLN:HA	2.32	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:385:ALA:CB	1:A:472:ARG:HG2	2.43	0.44
1:A:432:ASN:N	1:A:432:ASN:OD1	2.49	0.44
1:A:190:ASP:HB2	1:A:191:GLY:H	1.57	0.44
1:A:220:ALA:HB2	1:A:497:MET:SD	2.58	0.44
1:A:315:SER:CB	1:A:318:THR:O	2.65	0.44
1:A:187:THR:HG22	1:A:189:ASN:ND2	2.33	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:512:LYS:HG2	1:A:513:ASN:N	2.32	0.43
1:A:158:ASP:O	1:A:159:TRP:C	2.56	0.43
1:A:116:ASN:HB3	1:A:119:LEU:O	2.18	0.43
1:A:292:SER:HA	1:A:430:THR:OG1	2.18	0.43
1:A:388:SER:O	1:A:389:HIS:HB3	2.18	0.43
1:A:360:ASN:O	1:A:361:SER:CB	2.65	0.43
1:A:360:ASN:OD1	1:A:360:ASN:C	2.57	0.43
1:A:102:VAL:HG13	1:A:102:VAL:O	2.18	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:379:LEU:HD12	1:A:380:VAL:H	1.84	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:576:THR:HG22	1:A:577:VAL:O	2.19	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:112:LEU:HA	1:A:113:PRO:HD3	1.65	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:91:TRP:NE1	1:A:93:CYS:HB2	2.34	0.42
1:A:469:TRP:CD1	1:A:469:TRP:C	2.93	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: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:447:GLN:OE1	1:A:447:GLN:C	2.59	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
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:347:ARG:NH1	1:A:438:GLN:HB3	2.35	0.41
1:A:174:LEU:HB2	1:A:545:ILE:HG12	2.03	0.41
1:A:564:THR:HG22	1:A:565:SER:C	2.41	0.41
1:A:279:GLU:O	1:A:280:ASP:C	2.58	0.41
1:A:96:THR:O	1:A:102:VAL:HA	2.19	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:298:ASN:HA	1:A:299:PRO:HD3	1.77	0.41
1:A:109:THR:HB	1:A:232:VAL:HG22	2.03	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: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:215:TYR:CE1	1:A:217:LEU:HD12	2.55	0.41
1:A:163:ILE:HG13	1:A:591:THR:HA	2.02	0.41
1:A:341:LEU:O	1:A:467:MET:HA	2.21	0.41
1:A:349:GLN:HB3	1:A:399:GLN:OE1	2.21	0.41
1:A:563:TYR:C	1:A:563:TYR:CD2	2.93	0.41
1:A:552:GLU:O	1:A:553:ASN:CB	2.66	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: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:175:ASN:HD22	1:A:176:PHE:H	1.68	0.40
1:A:122:GLN:HG2	1:A:123:ILE:N	2.36	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%)	3 15

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	SER

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Mol	Chain	Res	Type
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%)	1 7

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
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

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Mol	Chain	Res	Type
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
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

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

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 ⓘ

There are no ligands in this entry.

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, 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	519/519 (100%)	-0.32	0 100 100	14, 23, 31, 42	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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.