



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:19 PM UTC

PDB ID : 1AKN / pdb_00001akn
Title : STRUCTURE OF BILE-SALT ACTIVATED LIPASE
Authors : Wang, X.; Zhang, X.
Deposited on : 1997-05-23
Resolution : 2.80 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
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

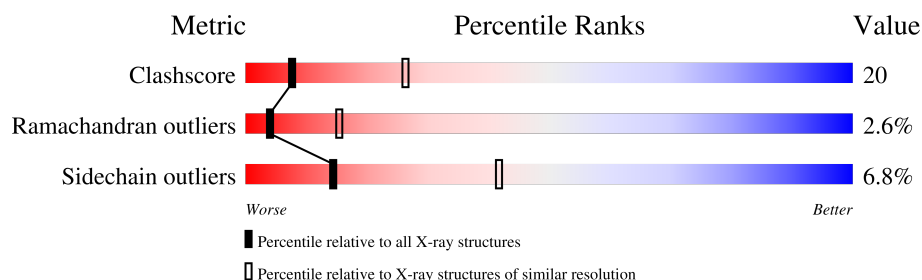
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	579	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 4275 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 BILE-SALT ACTIVATED LIPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	547	4261	2725	708	811	17	0	0	0

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



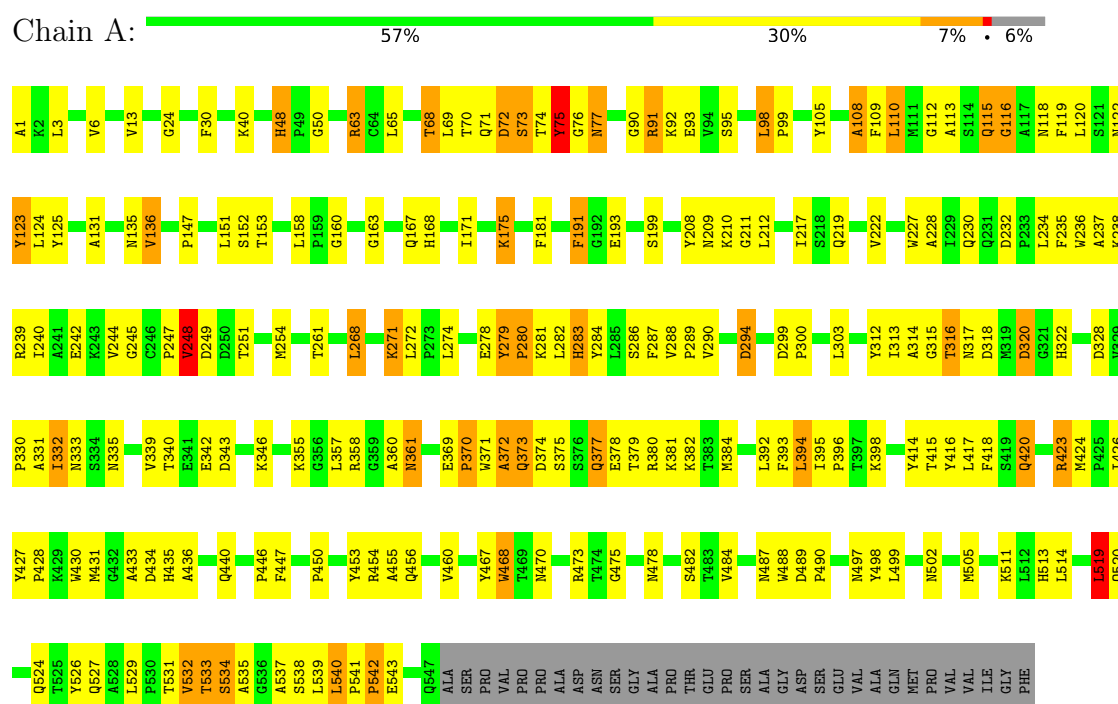
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0

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: BILE-SALT ACTIVATED LIPASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	94.39Å 94.39Å 144.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	95.3 (8.00-2.80)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.211 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4275	wwPDB-VP
Average B, all atoms (Å ²)	47.0	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:
NAG

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	0.52	0/4376	1.05	27/5959 (0.5%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	HIS	CA-C-N	8.42	128.06	119.56
1	A	48	HIS	C-N-CA	8.42	128.06	119.56
1	A	294	ASP	N-CA-C	8.20	123.21	112.72
1	A	73	SER	N-CA-C	-7.79	99.85	110.68
1	A	372	ALA	N-CA-C	-7.32	104.50	113.50
1	A	475	GLY	N-CA-C	-7.17	105.88	115.21
1	A	519	LEU	N-CA-C	-7.02	103.56	111.07
1	A	533	THR	N-CA-C	-6.69	104.02	111.71
1	A	361	ASN	CB-CG-ND2	6.48	126.12	116.40
1	A	394	LEU	N-CA-C	6.36	117.91	110.97
1	A	63	ARG	N-CA-C	-6.13	102.87	110.41
1	A	318	ASP	N-CA-C	5.87	119.97	112.34
1	A	513	HIS	N-CA-C	5.85	118.33	111.02
1	A	358	ARG	N-CA-C	-5.80	104.88	111.14
1	A	268	LEU	N-CA-C	5.79	118.37	111.71
1	A	158	LEU	CA-C-N	5.57	124.92	118.85
1	A	158	LEU	C-N-CA	5.57	124.92	118.85
1	A	470	ASN	N-CA-C	-5.25	105.45	111.07
1	A	286	SER	N-CA-C	5.24	116.99	111.28
1	A	542	PRO	N-CA-C	5.23	118.70	110.80
1	A	377	GLN	N-CA-C	-5.20	106.03	112.38
1	A	299	ASP	CA-C-N	5.17	125.46	119.47
1	A	299	ASP	C-N-CA	5.17	125.46	119.47
1	A	392	LEU	N-CA-C	5.11	118.66	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	PRO	N-CA-C	5.07	119.04	111.14
1	A	482	SER	N-CA-C	5.02	117.31	109.52
1	A	248	VAL	N-CA-C	5.01	119.76	109.34

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4261	0	4139	169	0
2	A	14	0	13	0	0
All	All	4275	0	4152	169	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 20.

All (169) 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:73:SER:HB3	1:A:268:LEU:HG	1.11	1.07
1:A:73:SER:HB3	1:A:268:LEU:CG	2.00	0.92
1:A:373:GLN:HG2	1:A:374:ASP:H	1.40	0.85
1:A:244:VAL:HG11	1:A:261:THR:HG21	1.57	0.84
1:A:227:TRP:O	1:A:288:VAL:HG21	1.84	0.78
1:A:300:PRO:HA	1:A:303:LEU:HD12	1.66	0.77
1:A:332:ILE:HG22	1:A:428:PRO:HD3	1.65	0.76
1:A:332:ILE:HG22	1:A:428:PRO:CD	2.17	0.74
1:A:288:VAL:HG22	1:A:289:PRO:HD2	1.71	0.73
1:A:467:TYR:CE1	1:A:484:VAL:HG13	2.24	0.71
1:A:119:PHE:HD1	1:A:120:LEU:H	1.39	0.70
1:A:427:TYR:HB3	1:A:431:MET:HG3	1.75	0.68
1:A:105:TYR:CE1	1:A:112:GLY:HA3	2.28	0.68
1:A:331:ALA:HB1	1:A:381:LYS:NZ	2.09	0.67
1:A:424:MET:HG3	1:A:426:ILE:HG12	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:SER:CB	1:A:268:LEU:HG	2.06	0.66
1:A:279:TYR:CD1	1:A:280:PRO:HD2	2.31	0.66
1:A:3:LEU:HD23	1:A:30:PHE:CZ	2.32	0.64
1:A:423:ARG:HA	1:A:423:ARG:HE	1.63	0.64
1:A:48:HIS:HD2	1:A:50:GLY:H	1.46	0.63
1:A:328:ASP:O	1:A:330:PRO:HD3	2.01	0.61
1:A:395:ILE:HB	1:A:396:PRO:HD3	1.82	0.61
1:A:320:ASP:HB3	1:A:393:PHE:CD2	2.35	0.61
1:A:288:VAL:HG22	1:A:289:PRO:CD	2.31	0.60
1:A:119:PHE:HD2	1:A:125:TYR:OH	1.85	0.60
1:A:531:THR:HG22	1:A:533:THR:N	2.17	0.60
1:A:537:ALA:O	1:A:542:PRO:HB2	2.01	0.59
1:A:63:ARG:HD2	1:A:75:TYR:HB3	1.84	0.59
1:A:416:TYR:HB3	1:A:488:TRP:CZ2	2.37	0.59
1:A:119:PHE:HB3	1:A:122:ASN:O	2.03	0.59
1:A:112:GLY:HA2	1:A:118:ASN:HB2	1.85	0.59
1:A:342:GLU:O	1:A:346:LYS:HD3	2.02	0.58
1:A:279:TYR:CG	1:A:280:PRO:HD2	2.37	0.58
1:A:478:ASN:HA	1:A:484:VAL:HG21	1.85	0.58
1:A:374:ASP:HA	1:A:380:ARG:CZ	2.33	0.58
1:A:68:THR:OG1	1:A:72:ASP:HB2	2.04	0.58
1:A:541:PRO:HB2	1:A:542:PRO:HD3	1.86	0.58
1:A:91:ARG:NE	1:A:91:ARG:H	2.01	0.57
1:A:116:GLY:HA3	1:A:124:LEU:HA	1.86	0.57
1:A:420:GLN:HG3	1:A:460:VAL:HG21	1.85	0.57
1:A:48:HIS:CD2	1:A:50:GLY:H	2.22	0.57
1:A:92:LYS:HG3	1:A:93:GLU:H	1.70	0.56
1:A:109:PHE:CD2	1:A:288:VAL:HG23	2.41	0.56
1:A:175:LYS:HG3	1:A:212:LEU:HD22	1.87	0.56
1:A:234:LEU:CD1	1:A:254:MET:HE1	2.36	0.55
1:A:339:VAL:HG11	1:A:384:MET:SD	2.47	0.55
1:A:3:LEU:HD23	1:A:30:PHE:HZ	1.72	0.55
1:A:446:PRO:HG3	1:A:453:TYR:CD1	2.42	0.55
1:A:340:THR:O	1:A:343:ASP:HB2	2.07	0.54
1:A:63:ARG:O	1:A:76:GLY:HA3	2.08	0.54
1:A:239:ARG:O	1:A:242:GLU:HB3	2.08	0.54
1:A:498:TYR:CE1	1:A:514:LEU:HB2	2.42	0.54
1:A:70:THR:HG23	1:A:71:GLN:N	2.22	0.54
1:A:373:GLN:HG2	1:A:374:ASP:N	2.16	0.53
1:A:91:ARG:NE	1:A:91:ARG:N	2.57	0.53
1:A:193:GLU:HA	1:A:219:GLN:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ALA:HB3	1:A:379:THR:HG21	1.91	0.53
1:A:99:PRO:HB2	1:A:136:VAL:HG22	1.92	0.52
1:A:312:TYR:CE2	1:A:314:ALA:HB2	2.44	0.52
1:A:447:PHE:O	1:A:450:PRO:HD3	2.10	0.52
1:A:153:THR:HG22	1:A:254:MET:HE3	1.91	0.52
1:A:230:GLN:HB3	1:A:290:VAL:HG12	1.91	0.52
1:A:230:GLN:HE21	1:A:232:ASP:H	1.57	0.52
1:A:24:GLY:HA3	1:A:91:ARG:HB3	1.92	0.51
1:A:70:THR:HG23	1:A:71:GLN:H	1.76	0.51
1:A:274:LEU:HD13	1:A:282:LEU:HD22	1.92	0.51
1:A:322:HIS:CE1	1:A:332:ILE:HG23	2.46	0.51
1:A:116:GLY:CA	1:A:124:LEU:HA	2.41	0.51
1:A:313:ILE:HA	1:A:414:TYR:O	2.11	0.51
1:A:339:VAL:N	1:A:377:GLN:OE1	2.44	0.51
1:A:535:ALA:HB1	1:A:538:SER:HB2	1.93	0.51
1:A:332:ILE:HG22	1:A:428:PRO:HD2	1.92	0.50
1:A:248:VAL:HG12	1:A:249:ASP:OD1	2.12	0.49
1:A:532:VAL:HG12	1:A:532:VAL:O	2.13	0.49
1:A:435:HIS:O	1:A:436:ALA:HB3	2.12	0.49
1:A:92:LYS:HG3	1:A:93:GLU:N	2.27	0.49
1:A:420:GLN:HG2	1:A:502:ASN:HA	1.95	0.49
1:A:315:GLY:HA3	1:A:416:TYR:CE2	2.48	0.49
1:A:77:ASN:H	1:A:77:ASN:HD22	1.60	0.49
1:A:355:LYS:HG3	1:A:526:TYR:CZ	2.48	0.49
1:A:468:TRP:N	1:A:468:TRP:HE3	2.12	0.48
1:A:113:ALA:HB1	1:A:115:GLN:HG2	1.96	0.48
1:A:122:ASN:OD1	1:A:440:GLN:HB3	2.12	0.48
1:A:152:SER:HB2	1:A:160:GLY:HA3	1.96	0.48
1:A:281:LYS:HD3	1:A:284:TYR:HB2	1.95	0.48
1:A:317:ASN:HA	1:A:418:PHE:O	2.14	0.48
1:A:77:ASN:ND2	1:A:77:ASN:N	2.62	0.48
1:A:235:PHE:HB3	1:A:236:TRP:CE3	2.49	0.48
1:A:478:ASN:HD22	1:A:484:VAL:HG11	1.79	0.48
1:A:75:TYR:HD1	1:A:75:TYR:HA	1.59	0.47
1:A:369:GLU:HB2	1:A:370:PRO:HD3	1.96	0.47
1:A:234:LEU:HG	1:A:238:LYS:HE2	1.97	0.47
1:A:272:LEU:HD22	1:A:274:LEU:HB2	1.97	0.47
1:A:71:GLN:O	1:A:268:LEU:HD21	2.14	0.47
1:A:416:TYR:HB3	1:A:488:TRP:HZ2	1.80	0.47
1:A:234:LEU:HA	1:A:237:ALA:HB3	1.97	0.46
1:A:478:ASN:HD21	1:A:488:TRP:H	1.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:TYR:CD1	1:A:123:TYR:N	2.84	0.46
1:A:228:ALA:O	1:A:289:PRO:HD2	2.16	0.46
1:A:238:LYS:HB3	1:A:248:VAL:HG13	1.97	0.46
1:A:478:ASN:ND2	1:A:484:VAL:HG11	2.31	0.46
1:A:478:ASN:ND2	1:A:487:ASN:HA	2.31	0.46
1:A:119:PHE:HD2	1:A:125:TYR:HH	1.63	0.46
1:A:191:PHE:HA	1:A:217:ILE:O	2.15	0.46
1:A:467:TYR:CE1	1:A:484:VAL:CG1	2.98	0.46
1:A:163:GLY:O	1:A:167:GLN:HG3	2.16	0.46
1:A:317:ASN:HB3	1:A:433:ALA:HB3	1.98	0.46
1:A:108:ALA:HB3	1:A:110:LEU:HD22	1.98	0.45
1:A:416:TYR:C	1:A:416:TYR:CD1	2.94	0.45
1:A:541:PRO:HD2	1:A:542:PRO:HD3	1.98	0.45
1:A:230:GLN:HB2	1:A:288:VAL:HG12	1.98	0.45
1:A:377:GLN:NE2	1:A:380:ARG:HD2	2.31	0.45
1:A:378:GLU:HG3	1:A:430:TRP:CD1	2.52	0.45
1:A:95:SER:HB3	1:A:98:LEU:HD22	1.98	0.45
1:A:235:PHE:C	1:A:235:PHE:CD1	2.94	0.45
1:A:281:LYS:HD3	1:A:284:TYR:CG	2.52	0.45
1:A:322:HIS:ND1	1:A:431:MET:SD	2.90	0.45
1:A:454:ARG:HB3	1:A:456:GLN:HG2	1.99	0.45
1:A:168:HIS:ND1	1:A:209:ASN:OD1	2.47	0.44
1:A:1:ALA:N	1:A:90:GLY:O	2.50	0.44
1:A:271:LYS:NZ	1:A:271:LYS:HB3	2.32	0.44
1:A:314:ALA:O	1:A:415:THR:HA	2.16	0.44
1:A:541:PRO:CB	1:A:542:PRO:HD3	2.47	0.44
1:A:135:ASN:O	1:A:473:ARG:NH2	2.50	0.44
1:A:454:ARG:HD2	1:A:455:ALA:H	1.82	0.44
1:A:77:ASN:HD22	1:A:77:ASN:N	2.14	0.44
1:A:316:THR:O	1:A:417:LEU:HD12	2.17	0.44
1:A:531:THR:C	1:A:533:THR:H	2.25	0.44
1:A:377:GLN:HE22	1:A:380:ARG:NH1	2.15	0.44
1:A:532:VAL:C	1:A:534:SER:N	2.74	0.44
1:A:70:THR:CG2	1:A:71:GLN:H	2.31	0.44
1:A:234:LEU:HD11	1:A:254:MET:HE1	2.00	0.44
1:A:210:LYS:HD3	1:A:211:GLY:N	2.32	0.43
1:A:108:ALA:HB3	1:A:110:LEU:CD2	2.48	0.43
1:A:489:ASP:HA	1:A:490:PRO:HD3	1.84	0.43
1:A:533:THR:O	1:A:534:SER:C	2.60	0.43
1:A:240:ILE:HG13	1:A:287:PHE:HZ	1.82	0.43
1:A:340:THR:OG1	1:A:342:GLU:HG2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ILE:HD12	1:A:519:LEU:HA	2.00	0.43
1:A:131:ALA:HA	1:A:136:VAL:O	2.18	0.43
1:A:244:VAL:HG11	1:A:261:THR:CG2	2.37	0.43
1:A:6:VAL:HG21	1:A:181:PHE:CE2	2.53	0.43
1:A:315:GLY:HA3	1:A:416:TYR:CZ	2.54	0.42
1:A:497:ASN:HA	1:A:511:LYS:O	2.19	0.42
1:A:70:THR:CG2	1:A:71:GLN:N	2.83	0.42
1:A:147:PRO:O	1:A:151:LEU:HB2	2.19	0.42
1:A:520:GLN:HG3	1:A:524:GLN:NE2	2.34	0.42
1:A:208:TYR:OH	1:A:294:ASP:HB2	2.19	0.42
1:A:240:ILE:HG13	1:A:287:PHE:CZ	2.55	0.41
1:A:499:LEU:HD11	1:A:505:MET:HE1	2.02	0.41
1:A:232:ASP:OD2	1:A:235:PHE:HB2	2.19	0.41
1:A:420:GLN:CG	1:A:460:VAL:HG21	2.51	0.41
1:A:40:LYS:HD2	1:A:40:LYS:HA	1.71	0.41
1:A:540:LEU:HB3	1:A:541:PRO:HD3	2.02	0.41
1:A:294:ASP:OD1	1:A:294:ASP:N	2.54	0.41
1:A:357:LEU:O	1:A:361:ASN:HB2	2.20	0.41
1:A:382:LYS:HE3	1:A:382:LYS:HB3	1.78	0.41
1:A:167:GLN:O	1:A:171:ILE:HG13	2.21	0.41
1:A:167:GLN:OE1	1:A:199:SER:HB3	2.21	0.41
1:A:72:ASP:C	1:A:74:THR:H	2.29	0.41
1:A:232:ASP:CG	1:A:235:PHE:HB2	2.46	0.41
1:A:112:GLY:HA2	1:A:118:ASN:CB	2.49	0.40
1:A:431:MET:HE1	1:A:434:ASP:HB2	2.04	0.40
1:A:537:ALA:C	1:A:539:LEU:H	2.29	0.40
1:A:357:LEU:HA	1:A:360:ALA:HB3	2.03	0.40
1:A:377:GLN:HA	1:A:380:ARG:HD2	2.04	0.40
1:A:478:ASN:ND2	1:A:488:TRP:H	2.19	0.40
1:A:394:LEU:O	1:A:398:LYS:HG3	2.21	0.40
1:A:333:ASN:O	1:A:335:ASN:N	2.53	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	545/579 (94%)	483 (89%)	48 (9%)	14 (3%)	4	15

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	HIS
1	A	68	THR
1	A	75	TYR
1	A	116	GLY
1	A	245	GLY
1	A	251	THR
1	A	72	ASP
1	A	108	ALA
1	A	373	GLN
1	A	534	SER
1	A	247	PRO
1	A	280	PRO
1	A	532	VAL
1	A	248	VAL

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	454/480 (95%)	423 (93%)	31 (7%)	14	42

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	65	LEU
1	A	69	LEU
1	A	75	TYR
1	A	77	ASN

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Mol	Chain	Res	Type
1	A	91	ARG
1	A	98	LEU
1	A	110	LEU
1	A	115	GLN
1	A	123	TYR
1	A	136	VAL
1	A	175	LYS
1	A	191	PHE
1	A	222	VAL
1	A	271	LYS
1	A	278	GLU
1	A	279	TYR
1	A	283	HIS
1	A	316	THR
1	A	320	ASP
1	A	332	ILE
1	A	371	TRP
1	A	375	SER
1	A	420	GLN
1	A	423	ARG
1	A	468	TRP
1	A	519	LEU
1	A	527	GLN
1	A	529	LEU
1	A	540	LEU
1	A	543	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	48	HIS
1	A	77	ASN
1	A	157	ASN
1	A	187	ASN
1	A	230	GLN
1	A	322	HIS
1	A	333	ASN
1	A	412	ASN
1	A	478	ASN
1	A	481	HIS
1	A	513	HIS

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Mol	Chain	Res	Type
1	A	520	GLN
1	A	524	GLN
1	A	545	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	NAG	A	600	1	14,14,15	0.96	0	17,19,21	1.15	2 (11%)

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	NAG	A	600	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	NAG	O5-C1-C2	-2.23	107.85	111.29
2	A	600	NAG	C8-C7-N2	-2.19	112.49	116.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.