WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2023 – 07:39 AM EDT

PDB ID	:	3K7L
Title	:	Structures of two elapid snake venom metalloproteases with distinct activities highlight the disulfide patterns in the D domain of ADAMalysin family proteins
Authors	:	Guan, H.H.; Wu, W.G.; Chen, C.J.
Deposited on	:	2009-10-13
Resolution	:	2.50 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

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 2.50 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	Percentile Ranks	Value
Rfree		0.230
Clashscore		24
Ramachandran outliers		0.5%
Sidechain outliers		15.3%
RSRZ outliers		2.2%

Worse *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
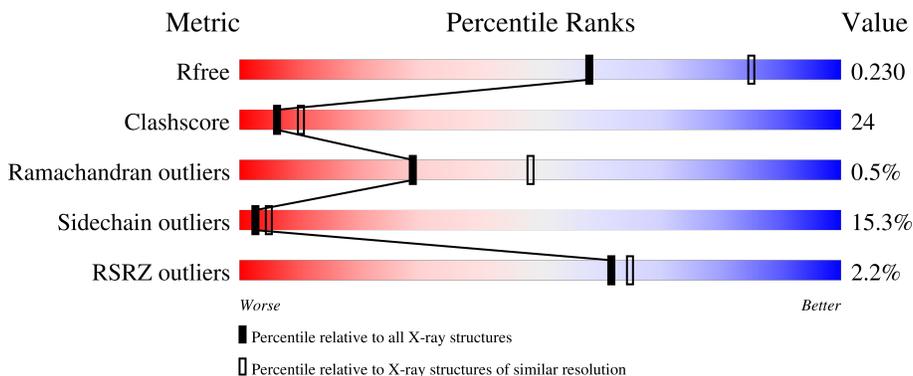
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	422	2% 58% 28% 9%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 3300 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 Atragin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total 3207	C 1970	N 588	O 601	S 48	0	0	0

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
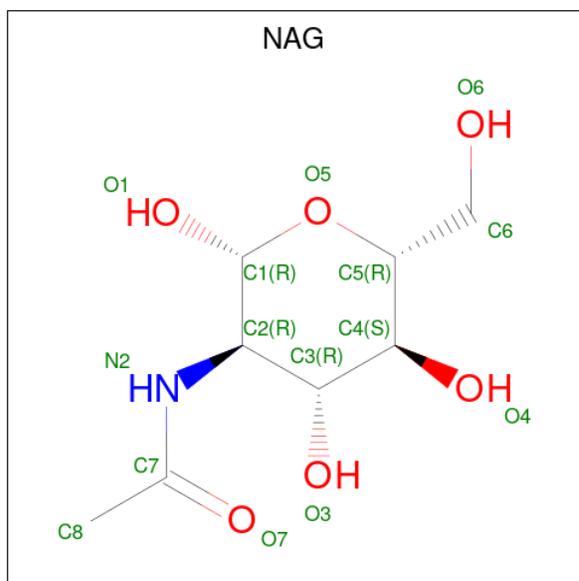
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Zn 1	0	0

• Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total 3	Ca 3	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	75	Total 75	O 75	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 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: Atragin
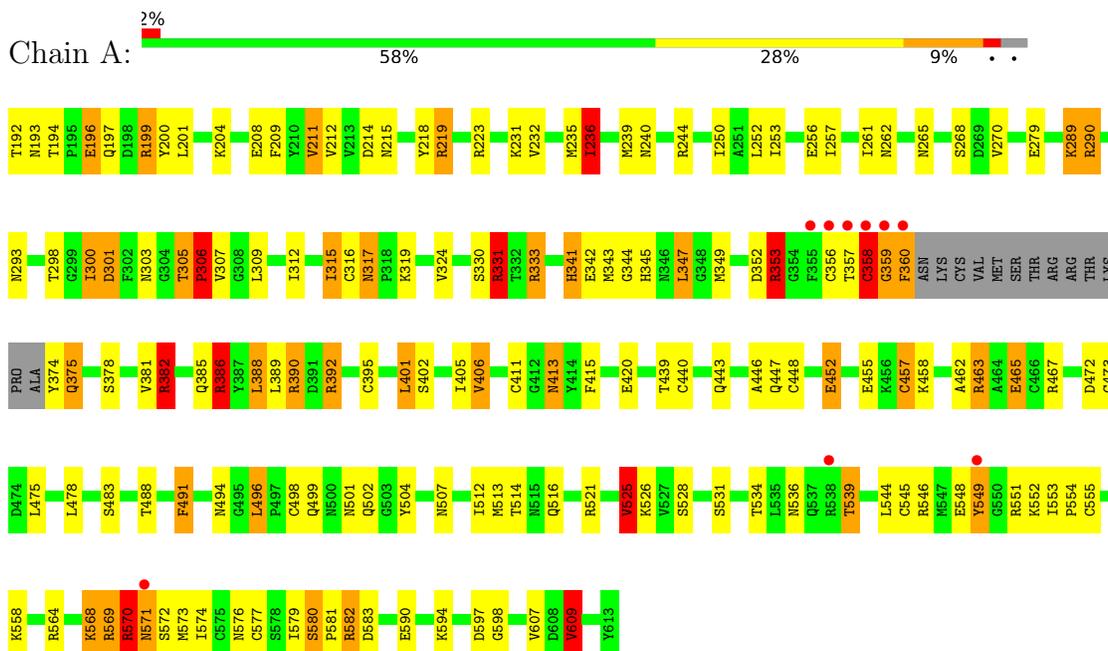
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	91.65Å 91.65Å 124.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 37.74 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.4 (30.00-2.50) 93.0 (37.74-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	4.93 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.234 0.223 , 0.230	Depositor DCC
R_{free} test set	2238 reflections (9.91%)	wwPDB-VP
Wilson B-factor (Å^2)	45.1	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 32.7	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3300	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, ZN, CA

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	1.55	24/3264 (0.7%)	1.40	31/4396 (0.7%)

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 (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	491	PHE	CE2-CZ	8.95	1.54	1.37
1	A	452	GLU	CB-CG	8.38	1.68	1.52
1	A	498	CYS	CB-SG	7.56	1.95	1.82
1	A	196	GLU	CG-CD	6.92	1.62	1.51
1	A	571	ASN	CB-CG	6.74	1.66	1.51
1	A	452	GLU	CG-CD	6.74	1.62	1.51
1	A	390	ARG	CG-CD	6.67	1.68	1.51
1	A	374	TYR	CE2-CZ	6.62	1.47	1.38
1	A	463	ARG	CB-CG	6.35	1.69	1.52
1	A	475	LEU	CG-CD2	6.10	1.74	1.51
1	A	549	TYR	CD2-CE2	5.99	1.48	1.39
1	A	491	PHE	CD1-CE1	5.57	1.50	1.39
1	A	330	SER	CB-OG	5.53	1.49	1.42
1	A	196	GLU	CD-OE2	5.52	1.31	1.25
1	A	609	VAL	CB-CG2	5.48	1.64	1.52
1	A	607	VAL	CB-CG1	5.38	1.64	1.52
1	A	199	ARG	CB-CG	5.38	1.67	1.52
1	A	411	CYS	CB-SG	5.36	1.91	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	TYR	CD2-CE2	5.35	1.47	1.39
1	A	465	GLU	CG-CD	5.24	1.59	1.51
1	A	395	CYS	CB-SG	5.11	1.91	1.82
1	A	279	GLU	CD-OE1	5.09	1.31	1.25
1	A	455	GLU	CB-CG	5.04	1.61	1.52
1	A	525	VAL	CB-CG1	5.03	1.63	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	ARG	NE-CZ-NH1	12.02	126.31	120.30
1	A	359	GLY	C-N-CA	-9.74	97.36	121.70
1	A	472	ASP	CB-CG-OD1	9.57	126.91	118.30
1	A	331	ARG	NE-CZ-NH2	-9.22	115.69	120.30
1	A	353	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	A	347	LEU	CB-CG-CD1	-9.00	95.70	111.00
1	A	359	GLY	N-CA-C	7.70	132.35	113.10
1	A	301	ASP	CB-CG-OD1	-7.57	111.48	118.30
1	A	467	ARG	NE-CZ-NH2	-7.17	116.71	120.30
1	A	293	ASN	CB-CA-C	6.92	124.24	110.40
1	A	352	ASP	N-CA-C	-6.82	92.58	111.00
1	A	331	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	A	467	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	A	496	LEU	CB-CG-CD1	-6.24	100.40	111.00
1	A	392	ARG	NE-CZ-NH2	6.19	123.39	120.30
1	A	406	VAL	CG1-CB-CG2	5.90	120.33	110.90
1	A	386	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	A	219	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	392	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	A	211	VAL	CB-CA-C	-5.68	100.61	111.40
1	A	401	LEU	CA-CB-CG	5.58	128.14	115.30
1	A	341	HIS	N-CA-CB	5.58	120.65	110.60
1	A	199	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	564	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	252	LEU	CB-CG-CD1	-5.36	101.89	111.00
1	A	382	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	236	ILE	CG1-CB-CG2	-5.20	99.95	111.40
1	A	244	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	301	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	472	ASP	CB-CG-OD2	-5.14	113.68	118.30
1	A	570	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	353	ARG	Peptide
1	A	357	THR	Peptide
1	A	358	CYS	Peptide

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	3207	0	3105	155	0
2	A	14	0	13	0	0
3	A	1	0	0	0	0
4	A	3	0	0	0	0
5	A	75	0	0	8	0
All	All	3300	0	3118	155	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 24.

All (155) 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:382:ARG:NH2	1:A:386:ARG:HG3	1.53	1.21
1:A:305:THR:HG22	1:A:306:PRO:HD3	1.17	1.16
1:A:359:GLY:O	1:A:360:PHE:C	1.74	1.14
1:A:569:ARG:HH12	1:A:570:ARG:HB3	1.24	1.02
1:A:341:HIS:CE1	1:A:353:ARG:NH2	2.29	1.00
1:A:240:ASN:HD21	1:A:250:ILE:H	1.03	0.99
1:A:215:ASN:H	1:A:262:ASN:HD21	1.02	0.95
1:A:462:ALA:O	1:A:463:ARG:HG2	1.66	0.94
1:A:382:ARG:NH2	1:A:386:ARG:CG	2.33	0.92
1:A:382:ARG:HH22	1:A:386:ARG:HG3	1.18	0.91
1:A:300:ILE:HD13	1:A:301:ASP:N	1.86	0.91
1:A:569:ARG:NH1	1:A:570:ARG:HB3	1.86	0.90
1:A:305:THR:HG22	1:A:306:PRO:CD	2.06	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ARG:HG2	1:A:333:ARG:NH2	1.91	0.85
1:A:305:THR:CG2	1:A:306:PRO:HD3	2.05	0.84
1:A:240:ASN:ND2	1:A:250:ILE:H	1.78	0.81
1:A:215:ASN:H	1:A:262:ASN:ND2	1.79	0.81
1:A:343:MET:O	1:A:347:LEU:HD12	1.80	0.81
1:A:494:ASN:HD21	1:A:507:ASN:H	1.28	0.80
1:A:331:ARG:HG2	1:A:333:ARG:HH21	1.45	0.80
1:A:525:VAL:HG23	1:A:569:ARG:HG2	1.63	0.80
1:A:317:ASN:HD22	1:A:319:LYS:H	1.31	0.79
1:A:381:VAL:O	1:A:385:GLN:HG3	1.83	0.79
1:A:315:ILE:HD13	1:A:316:CYS:N	1.98	0.78
1:A:465:GLU:HA	1:A:478:LEU:HD23	1.66	0.78
1:A:574:ILE:HD12	1:A:574:ILE:H	1.49	0.76
1:A:200:TYR:CD1	1:A:392:ARG:NH2	2.53	0.76
1:A:549:TYR:O	1:A:549:TYR:CD2	2.39	0.76
1:A:333:ARG:HD2	5:A:716:HOH:O	1.86	0.75
1:A:549:TYR:HE2	1:A:551:ARG:NH1	1.84	0.75
1:A:240:ASN:HD21	1:A:250:ILE:N	1.85	0.73
1:A:516:GLN:HE22	1:A:590:GLU:H	1.36	0.73
1:A:521:ARG:HH22	1:A:576:ASN:HB3	1.52	0.73
1:A:343:MET:O	1:A:347:LEU:CD1	2.38	0.72
1:A:236:ILE:HD13	1:A:239:MET:SD	2.31	0.71
1:A:569:ARG:HB2	5:A:772:HOH:O	1.91	0.70
1:A:569:ARG:NH1	1:A:570:ARG:H	1.90	0.69
1:A:300:ILE:HD13	1:A:301:ASP:H	1.57	0.69
1:A:194:THR:H	1:A:197:GLN:HE21	1.39	0.68
1:A:504:TYR:CE2	1:A:594:LYS:HE3	2.29	0.67
1:A:305:THR:H	1:A:306:PRO:HD2	1.59	0.67
1:A:402:SER:HA	1:A:405:ILE:HD12	1.76	0.66
1:A:317:ASN:ND2	1:A:319:LYS:H	1.93	0.66
1:A:516:GLN:CD	1:A:590:GLU:HG3	2.17	0.64
1:A:208:GLU:HB3	1:A:253:ILE:HD13	1.79	0.64
1:A:347:LEU:HD12	1:A:347:LEU:N	2.12	0.63
1:A:209:PHE:CD2	1:A:236:ILE:HD11	2.33	0.62
1:A:548:GLU:O	1:A:549:TYR:HB3	1.98	0.62
1:A:516:GLN:NE2	1:A:590:GLU:HG3	2.14	0.62
1:A:549:TYR:CE2	1:A:551:ARG:NH1	2.67	0.60
1:A:569:ARG:HH12	1:A:570:ARG:CB	2.08	0.60
1:A:569:ARG:N	5:A:772:HOH:O	2.35	0.60
1:A:317:ASN:HD22	1:A:319:LYS:N	1.98	0.60
1:A:268:SER:OG	1:A:300:ILE:HD11	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:ILE:HD13	1:A:316:CYS:H	1.67	0.59
1:A:341:HIS:CD2	1:A:341:HIS:O	2.55	0.59
1:A:343:MET:HG2	1:A:347:LEU:HD11	1.84	0.59
1:A:236:ILE:HD12	1:A:250:ILE:HG21	1.85	0.58
1:A:580:SER:HB3	1:A:583:ASP:H	1.67	0.58
1:A:548:GLU:HB3	1:A:553:ILE:CD1	2.34	0.58
1:A:192:THR:OG1	1:A:193:ASN:N	2.36	0.57
1:A:261:ILE:HD12	1:A:261:ILE:O	2.03	0.57
1:A:499:GLN:O	1:A:502:GLN:HB2	2.04	0.57
1:A:194:THR:N	1:A:197:GLN:HE21	2.03	0.56
1:A:512:ILE:HG22	1:A:514:THR:H	1.71	0.56
1:A:344:GLY:O	1:A:349:MET:HG3	2.05	0.55
1:A:569:ARG:CZ	1:A:570:ARG:HB3	2.35	0.55
1:A:305:THR:N	1:A:306:PRO:HD2	2.22	0.55
1:A:570:ARG:C	1:A:572:SER:H	2.10	0.54
1:A:579:ILE:HG22	1:A:580:SER:N	2.22	0.54
1:A:580:SER:CB	1:A:582:ARG:HG3	2.36	0.54
1:A:289:LYS:HE2	1:A:290:ARG:NH1	2.23	0.54
1:A:236:ILE:HD12	1:A:250:ILE:CG2	2.37	0.54
1:A:402:SER:HA	1:A:405:ILE:CD1	2.38	0.54
1:A:494:ASN:ND2	1:A:507:ASN:H	2.00	0.54
1:A:378:SER:O	1:A:381:VAL:HG22	2.07	0.54
1:A:549:TYR:CD2	1:A:551:ARG:HG2	2.43	0.54
1:A:382:ARG:HH22	1:A:386:ARG:CG	2.03	0.53
1:A:446:ALA:HB1	1:A:457:CYS:HB3	1.89	0.53
1:A:215:ASN:N	1:A:262:ASN:HD21	1.87	0.53
1:A:194:THR:H	1:A:197:GLN:NE2	2.07	0.53
1:A:312:ILE:HD13	1:A:345:HIS:HB3	1.91	0.53
1:A:215:ASN:ND2	1:A:219:ARG:HG3	2.24	0.52
1:A:232:VAL:O	1:A:235:MET:HB2	2.08	0.52
1:A:257:ILE:HD12	1:A:257:ILE:N	2.25	0.52
1:A:516:GLN:NE2	1:A:590:GLU:H	2.05	0.52
1:A:462:ALA:O	1:A:463:ARG:CG	2.47	0.52
1:A:447:GLN:O	1:A:448:CYS:HB3	2.10	0.52
1:A:569:ARG:CZ	1:A:570:ARG:H	2.23	0.52
1:A:549:TYR:O	1:A:549:TYR:CG	2.63	0.51
1:A:341:HIS:ND1	1:A:353:ARG:NH2	2.44	0.51
1:A:331:ARG:HH11	1:A:333:ARG:NH2	2.08	0.51
1:A:375:GLN:C	1:A:375:GLN:HE21	2.13	0.51
1:A:375:GLN:HB3	5:A:711:HOH:O	2.10	0.51
1:A:452:GLU:HG2	5:A:729:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ASN:HD21	1:A:319:LYS:HB2	1.77	0.50
1:A:534:THR:O	1:A:534:THR:HG22	2.10	0.50
1:A:209:PHE:HD2	1:A:236:ILE:HD11	1.76	0.49
1:A:548:GLU:HB3	1:A:553:ILE:HD12	1.95	0.49
1:A:388:LEU:O	1:A:392:ARG:HG2	2.12	0.49
1:A:569:ARG:CZ	1:A:570:ARG:N	2.75	0.49
1:A:598:GLY:O	1:A:609:VAL:HG22	2.13	0.49
1:A:231:LYS:O	1:A:235:MET:HG3	2.13	0.49
1:A:257:ILE:HD12	1:A:257:ILE:H	1.78	0.49
1:A:569:ARG:NH2	1:A:570:ARG:HB3	2.28	0.48
1:A:208:GLU:HB3	1:A:253:ILE:CD1	2.43	0.48
1:A:548:GLU:O	1:A:549:TYR:CB	2.61	0.48
1:A:504:TYR:HE2	1:A:594:LYS:HG3	1.78	0.47
1:A:289:LYS:HE2	1:A:290:ARG:HH12	1.78	0.47
1:A:270:VAL:HG13	1:A:309:LEU:HD22	1.97	0.47
1:A:420:GLU:HG2	5:A:725:HOH:O	2.15	0.47
1:A:420:GLU:CG	5:A:725:HOH:O	2.63	0.46
1:A:465:GLU:CA	1:A:478:LEU:HD23	2.43	0.46
1:A:569:ARG:HH22	1:A:570:ARG:HB3	1.80	0.46
1:A:473:CYS:O	1:A:491:PHE:HB3	2.16	0.46
1:A:580:SER:OG	1:A:582:ARG:HG3	2.16	0.46
1:A:539:THR:HG23	1:A:539:THR:O	2.16	0.45
1:A:569:ARG:NH1	1:A:570:ARG:N	2.62	0.45
1:A:250:ILE:N	1:A:250:ILE:HD12	2.31	0.45
1:A:413:ASN:HD22	1:A:413:ASN:C	2.18	0.45
1:A:539:THR:O	1:A:539:THR:CG2	2.65	0.45
1:A:553:ILE:HA	1:A:554:PRO:HD2	1.59	0.45
1:A:375:GLN:NE2	1:A:375:GLN:CA	2.80	0.44
1:A:305:THR:CG2	1:A:306:PRO:CD	2.81	0.44
1:A:405:ILE:CD1	1:A:415:PHE:HE1	2.30	0.44
1:A:570:ARG:HD3	1:A:571:ASN:H	1.81	0.44
1:A:342:GLU:HA	1:A:342:GLU:OE2	2.18	0.44
1:A:534:THR:O	1:A:534:THR:CG2	2.66	0.44
1:A:375:GLN:HE21	1:A:375:GLN:CA	2.31	0.43
1:A:536:ASN:HB3	1:A:555:CYS:SG	2.57	0.43
1:A:583:ASP:C	1:A:583:ASP:OD2	2.56	0.43
1:A:579:ILE:CG2	1:A:580:SER:N	2.81	0.43
1:A:570:ARG:C	1:A:572:SER:N	2.72	0.43
1:A:516:GLN:NE2	1:A:590:GLU:CG	2.81	0.43
1:A:568:LYS:HD2	1:A:569:ARG:O	2.18	0.43
1:A:571:ASN:O	1:A:572:SER:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:SER:HA	1:A:581:PRO:HD2	1.87	0.42
1:A:439:THR:O	1:A:440:CYS:HB2	2.19	0.42
1:A:446:ALA:CB	1:A:457:CYS:HB3	2.49	0.42
1:A:512:ILE:O	1:A:513:MET:C	2.55	0.42
1:A:568:LYS:O	1:A:568:LYS:HG3	2.19	0.42
1:A:315:ILE:O	1:A:316:CYS:HB2	2.19	0.42
1:A:211:VAL:HG12	1:A:212:VAL:N	2.34	0.41
1:A:504:TYR:CZ	1:A:594:LYS:HE3	2.55	0.41
1:A:215:ASN:HD21	1:A:219:ARG:HG3	1.86	0.41
1:A:413:ASN:ND2	1:A:415:PHE:H	2.19	0.41
1:A:573:MET:HE3	5:A:752:HOH:O	2.21	0.41
1:A:577:CYS:SG	1:A:579:ILE:HD11	2.60	0.41
1:A:240:ASN:HD21	1:A:250:ILE:HB	1.86	0.41
1:A:194:THR:OG1	1:A:197:GLN:HG3	2.21	0.41
1:A:386:ARG:HD3	1:A:390:ARG:HH21	1.85	0.41
1:A:305:THR:N	1:A:306:PRO:CD	2.84	0.41
1:A:219:ARG:HH11	1:A:223:ARG:NE	2.19	0.40
1:A:211:VAL:CG1	1:A:212:VAL:N	2.83	0.40
1:A:539:THR:HG23	1:A:552:LYS:HD2	2.03	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	405/422 (96%)	367 (91%)	36 (9%)	2 (0%)	29	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	358	CYS
1	A	306	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	359/371 (97%)	304 (85%)	55 (15%)	2 5

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	GLU
1	A	199	ARG
1	A	201	LEU
1	A	204	LYS
1	A	214	ASP
1	A	236	ILE
1	A	256	GLU
1	A	265	ASN
1	A	289	LYS
1	A	290	ARG
1	A	298	THR
1	A	300	ILE
1	A	303	ASN
1	A	305	THR
1	A	306	PRO
1	A	307	VAL
1	A	315	ILE
1	A	317	ASN
1	A	324	VAL
1	A	331	ARG
1	A	333	ARG
1	A	356	CYS
1	A	358	CYS
1	A	360	PHE
1	A	375	GLN
1	A	382	ARG
1	A	386	ARG
1	A	388	LEU
1	A	389	LEU
1	A	401	LEU

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Mol	Chain	Res	Type
1	A	406	VAL
1	A	413	ASN
1	A	443	GLN
1	A	457	CYS
1	A	458	LYS
1	A	483	SER
1	A	488	THR
1	A	496	LEU
1	A	501	ASN
1	A	525	VAL
1	A	526	LYS
1	A	528	SER
1	A	531	SER
1	A	539	THR
1	A	544	LEU
1	A	545	CYS
1	A	546	ARG
1	A	558	LYS
1	A	568	LYS
1	A	569	ARG
1	A	570	ARG
1	A	580	SER
1	A	582	ARG
1	A	597	ASP
1	A	609	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	GLN
1	A	215	ASN
1	A	240	ASN
1	A	260	ASN
1	A	262	ASN
1	A	265	ASN
1	A	293	ASN
1	A	295	GLN
1	A	317	ASN
1	A	326	GLN
1	A	345	HIS
1	A	346	ASN
1	A	350	ASN

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Mol	Chain	Res	Type
1	A	351	HIS
1	A	375	GLN
1	A	443	GLN
1	A	492	GLN
1	A	494	ASN
1	A	515	ASN
1	A	516	GLN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

5.4   Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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	1	1	14,14,15	1.15	1 (7%)	17,19,21	2.28	4 (23%)

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	1	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	NAG	C4-C5	2.46	1.58	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	NAG	C4-C3-C2	-6.00	102.22	111.02
2	A	1	NAG	C3-C4-C5	-3.67	103.69	110.24
2	A	1	NAG	O4-C4-C5	3.33	117.56	109.30
2	A	1	NAG	O4-C4-C3	2.54	116.23	110.35

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	NAG	O5-C5-C6-O6
2	A	1	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	409/422 (96%)	-0.28	9 (2%)	62	65	28, 45, 81, 153	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	360	PHE	9.8
1	A	359	GLY	7.6
1	A	549	TYR	4.2
1	A	355	PHE	4.0
1	A	357	THR	3.8
1	A	358	CYS	3.7
1	A	356	CYS	3.3
1	A	571	ASN	3.0
1	A	538	ARG	2.1

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 monosaccharides 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. The B-factors column lists the minimum, median, 95th 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	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	A	1	14/15	0.90	0.14	70,74,81,84	0
4	CA	A	701	1/1	0.93	0.07	57,57,57,57	0
4	CA	A	702	1/1	0.96	0.10	45,45,45,45	0
3	ZN	A	704	1/1	0.97	0.28	107,107,107,107	0
4	CA	A	703	1/1	0.98	0.08	34,34,34,34	0

6.5 Other polymers ⓘ

There are no such residues in this entry.