



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 06:16 PM GMT

PDB ID : 3DSL
Title : The Three-dimensional Structure of Bothropasin, the Main Hemorrhagic Factor from Bothrops jararaca venom.
Authors : Muniz, J.R.C.; Ambrosio, A.; Selistre-de-Araujo, H.S.; Oliva, G.; Garratt, R.C.; Souza, D.H.F.
Deposited on : 2008-07-13
Resolution : 2.70 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>

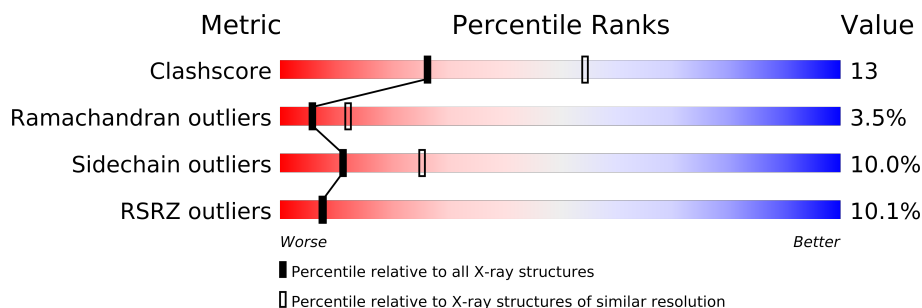
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.70 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	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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	419	
1	B	419	

2 Entry composition i

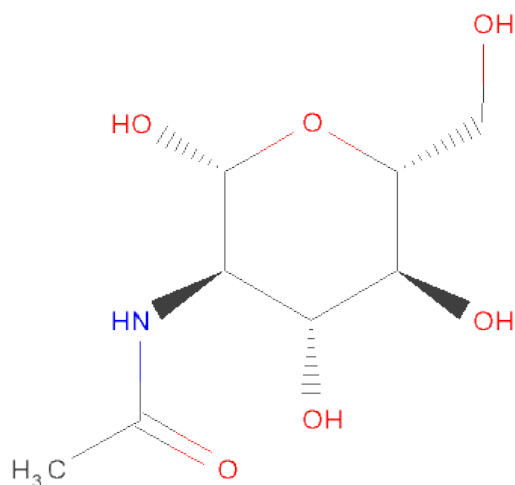
There are 6 unique types of molecules in this entry. The entry contains 6675 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Zinc metalloproteinase-disintegrinbothropasin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3219	1998	543	631	47			
1	B	412	Total	C	N	O	S	0	0	0
			3190	1981	538	624	47			

- Molecule 2 is Polymer: 2 Molecule: Bothropasin Chains: B (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Ca	0	0
			3	3		

Continued on next page...

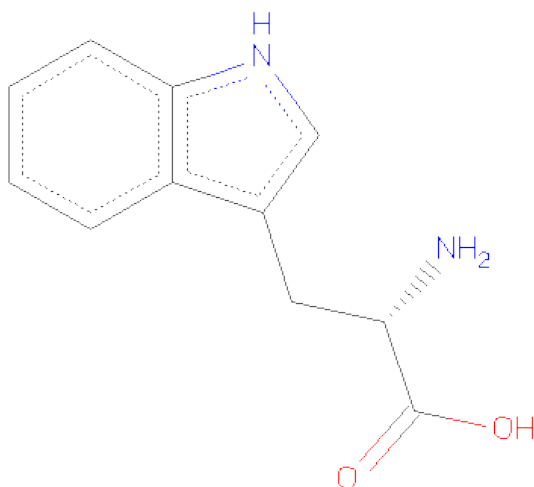
Continued from previous page...

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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is FUROYL-LEUCINE (three-letter code: TRP, FLE) (formula: $C_{11}H_{12}N_2O_2$, $C_{11}H_{15}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	4	Total	C	N	O	0	0
			60	44	6	10		

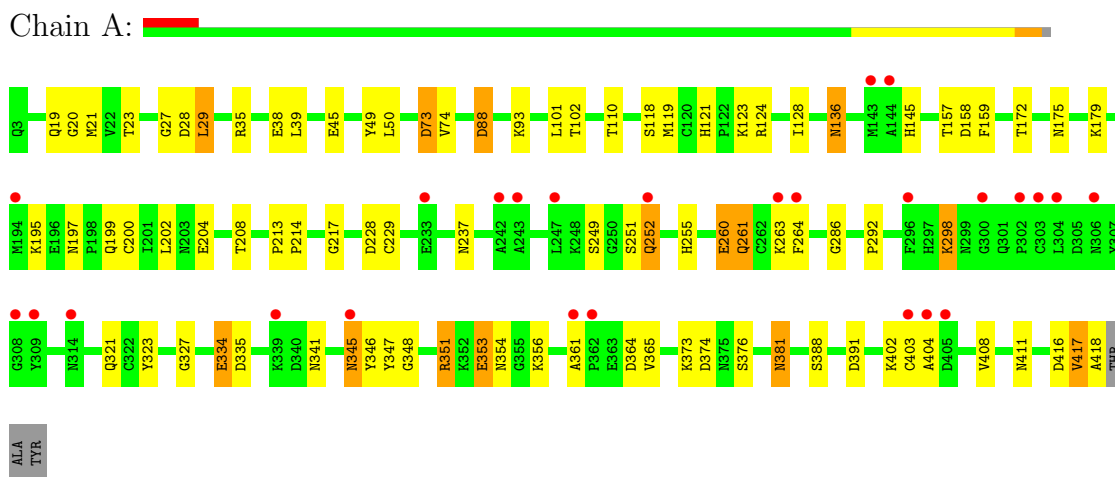
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	113	Total	O	0	0
			113	113		
6	B	71	Total	O	0	0
			71	71		

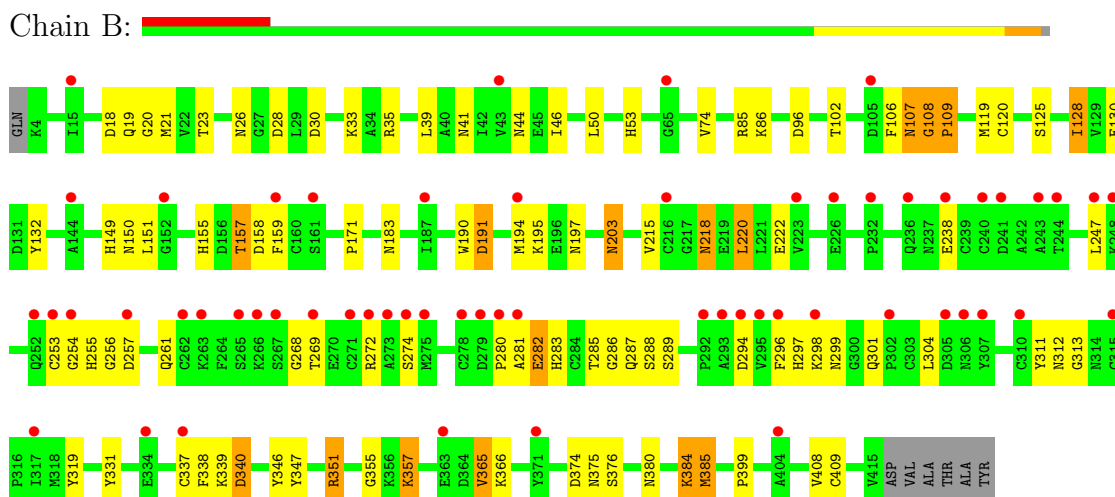
3 Residue-property plots

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: Zinc metalloproteinase-disintegrinbothropasin



- Molecule 1: Zinc metalloproteinase-disintegrinbothropasin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.76Å 100.27Å 133.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.44 – 2.70 30.44 – 2.70	Depositor EDS
% Data completeness (in resolution range)	88.9 (30.44-2.70) 92.0 (30.44-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.210 , 0.294 0.230 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 25588 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6675	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, FLE, CA, 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	0.42	0/3294	0.58	0/4458
1	B	0.43	1/3265 (0.0%)	0.58	1/4418 (0.0%)
All	All	0.43	1/6559 (0.0%)	0.58	1/8876 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	355	GLY	C-N	-12.36	1.05	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	355	GLY	O-C-N	5.76	131.91	122.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3219	0	29	42	0
1	B	3190	0	30	46	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	14	0	13	1	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	60	0	48	2	0
6	A	113	0	0	5	0
6	B	71	0	0	3	0
All	All	6675	0	120	88	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 13.

All (88) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:357:LYS:N	1:B:357:LYS:HD3	1.52	1.13
1:B:357:LYS:N	1:B:357:LYS:CD	2.29	0.85
1:A:353:GLU:OE1	1:A:353:GLU:CA	2.30	0.79
1:A:121:HIS:CD2	1:A:123:LYS:N	2.60	0.69
1:A:356:LYS:HD3	1:A:356:LYS:N	2.08	0.68
1:B:297:HIS:ND1	1:B:301:GLN:OE1	2.31	0.64
1:B:255:HIS:CG	1:B:256:GLY:N	2.67	0.62
1:A:260:GLU:O	1:A:261:GLN:C	2.40	0.59
1:B:33:LYS:NZ	6:B:449:HOH:O	2.36	0.58
1:B:282:GLU:OE1	1:B:294:ASP:OD1	2.21	0.58
1:A:204:GLU:OE2	1:A:255:HIS:NE2	2.37	0.58
1:A:388:SER:N	6:A:532:HOH:O	2.37	0.57
1:A:73:ASP:OD2	1:A:73:ASP:O	2.22	0.57
1:B:280:PRO:O	1:B:282:GLU:N	2.37	0.57
1:A:88:ASP:OD2	1:A:88:ASP:C	2.44	0.56
1:B:408:VAL:CG1	1:B:409:CYS:N	2.69	0.55
1:B:286:GLY:C	1:B:288:SER:N	2.61	0.54
1:A:381:ASN:C	1:A:381:ASN:ND2	2.62	0.52
1:B:203:ASN:ND2	1:B:203:ASN:N	2.57	0.52
1:B:106:PHE:CZ	1:B:128:ILE:CD1	2.93	0.52
1:B:190:TRP:O	1:B:194:MET:N	2.44	0.51
1:B:218:ASN:ND2	1:B:220:LEU:N	2.59	0.51
1:A:356:LYS:CD	1:A:356:LYS:N	2.74	0.51
1:A:136:ASN:N	1:A:136:ASN:ND2	2.58	0.50
1:A:45:GLU:OE2	1:A:179:LYS:NZ	2.44	0.50
1:A:334:GLU:N	1:A:334:GLU:CD	2.64	0.50
1:A:335:ASP:N	6:A:522:HOH:O	2.44	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:311:TYR:O	1:B:313:GLY:N	2.44	0.49
1:B:286:GLY:O	1:B:288:SER:N	2.44	0.49
1:B:107:ASN:O	1:B:108:GLY:C	2.49	0.49
1:A:345:ASN:ND2	1:A:345:ASN:N	2.60	0.49
1:A:374:ASP:OD1	1:A:376:SER:N	2.46	0.48
1:A:145:HIS:CE1	5:A:505:TRP:CE2	3.02	0.48
1:B:157:THR:OG1	1:B:158:ASP:N	2.46	0.48
1:A:217:GLY:N	1:A:228:ASP:OD2	2.47	0.48
1:A:351:ARG:NH1	1:A:351:ARG:CG	2.76	0.47
1:A:345:ASN:O	1:A:347:TYR:N	2.47	0.47
1:A:159:PHE:O	2:A:501:NAG:H3	2.13	0.47
1:B:149:HIS:O	1:B:151:LEU:N	2.47	0.47
1:B:346:TYR:N	6:B:467:HOH:O	2.47	0.47
1:A:286:GLY:N	6:A:544:HOH:O	2.48	0.47
1:B:218:ASN:ND2	1:B:218:ASN:C	2.68	0.47
1:A:118:SER:O	1:A:119:MET:C	2.51	0.47
1:A:229:CYS:N	6:A:517:HOH:O	2.47	0.47
1:B:337:CYS:O	1:B:339:LYS:N	2.48	0.47
1:A:73:ASP:C	1:A:73:ASP:OD2	2.54	0.46
1:A:252:GLN:NE2	1:A:264:PHE:N	2.64	0.46
1:B:19:GLN:O	1:B:20:GLY:C	2.52	0.46
1:B:319:TYR:CE1	1:B:331:TYR:CD2	3.03	0.46
1:B:183:ASN:ND2	6:B:484:HOH:O	2.48	0.46
1:B:107:ASN:O	1:B:109:PRO:N	2.50	0.45
1:B:385:MET:C	1:B:385:MET:SD	2.95	0.45
1:B:44:ASN:ND2	1:B:53:HIS:CD2	2.85	0.45
1:B:375:ASN:O	1:B:376:SER:C	2.56	0.44
1:B:285:THR:C	1:B:286:GLY:O	2.54	0.44
1:B:119:MET:O	1:B:120:CYS:CB	2.65	0.44
5:A:506:FLE:HG	1:B:109:PRO:O	2.18	0.44
1:B:191:ASP:O	1:B:195:LYS:N	2.50	0.44
1:A:347:TYR:CD1	1:A:348:GLY:N	2.86	0.44
1:B:96:ASP:O	1:B:125:SER:OG	2.36	0.43
1:A:417:VAL:CG1	1:A:418:ALA:N	2.82	0.43
1:A:19:GLN:O	1:A:20:GLY:C	2.58	0.43
1:A:298:LYS:CD	1:A:298:LYS:N	2.82	0.43
1:A:252:GLN:NE2	1:A:264:PHE:CG	2.87	0.43
1:B:130:GLU:O	1:B:132:TYR:N	2.52	0.43
1:A:49:TYR:N	6:A:568:HOH:O	2.52	0.43
1:A:121:HIS:CE1	1:A:124:ARG:NH1	2.87	0.42
1:A:323:TYR:O	1:A:327:GLY:N	2.52	0.42
1:B:296:PHE:O	1:B:297:HIS:CD2	2.72	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:157:THR:O	1:A:158:ASP:C	2.57	0.42
1:B:155:HIS:CD2	1:B:171:PRO:CA	3.02	0.42
1:A:341:ASN:OD1	1:A:365:VAL:O	2.37	0.42
1:B:23:THR:O	1:B:26:ASN:N	2.53	0.42
1:B:215:VAL:N	1:B:222:GLU:OE1	2.53	0.42
1:B:337:CYS:C	1:B:339:LYS:N	2.73	0.42
1:A:35:ARG:NE	1:A:136:ASN:OD1	2.52	0.42
1:B:149:HIS:C	1:B:151:LEU:N	2.73	0.41
1:A:27:GLY:O	1:A:29:LEU:N	2.53	0.41
1:A:101:LEU:CD1	1:A:101:LEU:N	2.83	0.41
1:B:215:VAL:CB	1:B:218:ASN:OD1	2.69	0.41
1:B:268:GLY:O	1:B:283:HIS:ND1	2.53	0.41
1:A:213:PRO:O	1:A:214:PRO:C	2.57	0.41
1:B:365:VAL:CG1	1:B:366:LYS:N	2.84	0.41
1:A:402:LYS:CE	1:A:404:ALA:O	2.69	0.40
1:B:108:GLY:O	1:B:109:PRO:C	2.60	0.40
1:B:374:ASP:OD2	1:B:384:LYS:NZ	2.54	0.40
1:B:340:ASP:OD2	1:B:347:TYR:OH	2.39	0.40
1:A:361:ALA:O	1:A:364:ASP:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	414/419 (99%)	351 (85%)	54 (13%)	9 (2%)	10	25
1	B	410/419 (98%)	320 (78%)	70 (17%)	20 (5%)	3	6
All	All	824/838 (98%)	671 (81%)	124 (15%)	29 (4%)	6	12

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	249	SER
1	B	107	ASN
1	B	157	THR
1	B	281	ALA
1	B	312	ASN
1	A	261	GLN
1	A	391	ASP
1	B	109	PRO
1	B	150	ASN
1	B	247	LEU
1	B	261	GLN
1	B	338	PHE
1	A	346	TYR
1	A	417	VAL
1	B	254	GLY
1	B	269	THR
1	A	292	PRO
1	B	304	LEU
1	B	351	ARG
1	B	399	PRO
1	A	197	ASN
1	B	28	ASP
1	B	282	GLU
1	B	298	LYS
1	A	411	ASN
1	B	46	ILE
1	B	287	GLN
1	B	108	GLY

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	361/363 (99%)	323 (90%)	38 (10%)	10	22
1	B	358/363 (99%)	326 (91%)	32 (9%)	14	31
All	All	719/726 (99%)	649 (90%)	70 (10%)	11	27

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	MET
1	A	23	THR
1	A	29	LEU
1	A	38	GLU
1	A	39	LEU
1	A	50	LEU
1	A	73	ASP
1	A	74	VAL
1	A	88	ASP
1	A	93	LYS
1	A	102	THR
1	A	110	THR
1	A	128	ILE
1	A	136	ASN
1	A	172	THR
1	A	175	ASN
1	A	195	LYS
1	A	199	GLN
1	A	200	CYS
1	A	202	LEU
1	A	208	THR
1	A	237	ASN
1	A	251	SER
1	A	252	GLN
1	A	260	GLU
1	A	263	LYS
1	A	298	LYS
1	A	321	GLN
1	A	334	GLU
1	A	345	ASN
1	A	351	ARG
1	A	353	GLU
1	A	354	ASN
1	A	373	LYS
1	A	381	ASN
1	A	403	CYS
1	A	408	VAL
1	A	416	ASP
1	B	18	ASP
1	B	21	MET
1	B	30	ASP
1	B	35	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	39	LEU
1	B	41	ASN
1	B	50	LEU
1	B	74	VAL
1	B	85	ARG
1	B	86	LYS
1	B	102	THR
1	B	128	ILE
1	B	159	PHE
1	B	191	ASP
1	B	197	ASN
1	B	203	ASN
1	B	218	ASN
1	B	220	LEU
1	B	238	GLU
1	B	253	CYS
1	B	257	ASP
1	B	272	ARG
1	B	274	SER
1	B	289	SER
1	B	299	ASN
1	B	340	ASP
1	B	351	ARG
1	B	357	LYS
1	B	365	VAL
1	B	380	ASN
1	B	384	LYS
1	B	385	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

Of 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 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	501	1	12,14,15	1.37	2 (16%)	15,19,21	1.26	1 (6%)
5	FLE	A	504	5	15,15,16	4.47	5 (33%)	15,19,21	3.58	5 (33%)
5	TRP	A	505	5,4	16,16,16	0.76	0	22,22,22	1.25	3 (13%)
5	FLE	A	506	5	15,15,16	4.08	5 (33%)	15,19,21	2.81	3 (20%)
5	TRP	A	507	5,4	16,16,16	0.75	1 (6%)	22,22,22	0.99	1 (4%)

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	501	1	-	0/6/23/26	0/1/1/1
5	FLE	A	504	5	-	0/10/14/16	0/1/1/1
5	TRP	A	505	5,4	-	0/8/8/8	0/0/2/2
5	FLE	A	506	5	-	0/10/14/16	0/1/1/1
5	TRP	A	507	5,4	-	0/8/8/8	0/0/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	504	FLE	O-C	15.67	1.22	1.11
5	A	506	FLE	O-C	13.89	1.20	1.11
5	A	504	FLE	CB-CA	4.51	1.58	1.53
5	A	506	FLE	CB-CA	4.26	1.57	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	506	FLE	C2-N	3.50	1.41	1.34
5	A	504	FLE	CA-N	3.25	1.50	1.46
5	A	504	FLE	CA-C	3.07	1.54	1.48
5	A	504	FLE	C2-N	3.02	1.40	1.34
5	A	506	FLE	CA-N	2.99	1.49	1.46
5	A	506	FLE	CA-C	2.65	1.53	1.48
2	A	501	NAG	C3-C2	2.45	1.57	1.52
2	A	501	NAG	O5-C5	-2.07	1.41	1.45
5	A	507	TRP	OXT-C	-2.04	1.23	1.30

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	506	FLE	C7-O8-C4	8.23	108.14	106.42
5	A	504	FLE	C7-O8-C4	8.12	108.12	106.42
5	A	504	FLE	C4-C2-N	8.07	130.58	116.89
5	A	506	FLE	C4-C2-N	5.11	125.56	116.89
5	A	504	FLE	CB-CA-N	4.53	120.65	109.97
5	A	504	FLE	O3-C2-N	-4.36	114.56	122.44
5	A	506	FLE	O3-C2-N	-3.82	115.54	122.44
5	A	504	FLE	CA-N-C2	-3.74	114.58	122.09
5	A	505	TRP	OXT-C-O	-3.28	116.66	124.07
5	A	505	TRP	C-CA-N	3.05	114.41	109.36
5	A	507	TRP	OXT-C-O	-2.89	117.53	124.07
2	A	501	NAG	C3-C4-C5	-2.69	105.41	110.20
5	A	505	TRP	O-C-CA	2.10	124.42	118.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	416/419 (99%)	0.32	26 (6%) 19 21	22, 38, 78, 180	0
1	B	412/419 (98%)	0.73	59 (14%) 3 4	24, 49, 129, 235	0
All	All	828/838 (98%)	0.52	85 (10%) 7 7	22, 43, 105, 235	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	248	LYS	6.4
1	B	273	ALA	6.2
1	A	404	ALA	6.1
1	B	267	SER	6.1
1	B	240	CYS	5.7
1	B	306	ASN	5.4
1	A	308	GLY	5.2
1	B	244	THR	5.0
1	B	280	PRO	4.8
1	B	262	CYS	4.8
1	A	361	ALA	4.8
1	B	247	LEU	4.5
1	B	279	ASP	4.4
1	B	296	PHE	4.4
1	B	293	ALA	4.3
1	B	238	GLU	4.2
1	A	296	PHE	4.1
1	A	194	MET	3.8
1	B	281	ALA	3.8
1	B	161	SER	3.7
1	B	257	ASP	3.6
1	B	187	ILE	3.5
1	B	223	VAL	3.5
1	B	263	LYS	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	266	LYS	3.4
1	B	275	MET	3.4
1	A	309	TYR	3.3
1	B	226	GLU	3.2
1	B	159	PHE	3.1
1	B	253	CYS	3.1
1	B	271	CYS	3.1
1	A	144	ALA	3.1
1	B	252	GLN	3.1
1	B	194	MET	3.0
1	B	404	ALA	3.0
1	A	304	LEU	2.9
1	B	278	CYS	2.9
1	A	300	GLY	2.8
1	B	363	GLU	2.8
1	B	334	GLU	2.8
1	A	314	ASN	2.7
1	B	310	CYS	2.7
1	B	295	VAL	2.6
1	B	298	LYS	2.6
1	B	302	PRO	2.6
1	A	252	GLN	2.6
1	B	269	THR	2.6
1	B	315	CYS	2.6
1	B	272	ARG	2.5
1	A	242	ALA	2.5
1	A	405	ASP	2.5
1	B	144	ALA	2.5
1	A	263	LYS	2.5
1	A	243	ALA	2.5
1	A	264	PHE	2.5
1	B	254	GLY	2.5
1	B	307	TYR	2.5
1	B	371	TYR	2.5
1	A	247	LEU	2.4
1	A	339	LYS	2.4
1	A	403	CYS	2.4
1	B	15	ILE	2.4
1	B	337	CYS	2.3
1	A	303	CYS	2.3
1	B	292	PRO	2.3
1	B	305	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	306	ASN	2.2
1	B	232	PRO	2.2
1	B	236	GLN	2.2
1	A	143	MET	2.2
1	B	265	SER	2.2
1	B	274	SER	2.1
1	B	317	ILE	2.1
1	B	105	ASP	2.1
1	A	345	ASN	2.1
1	A	302	PRO	2.1
1	A	362	PRO	2.1
1	B	243	ALA	2.1
1	B	216	CYS	2.1
1	B	294	ASP	2.1
1	B	241	ASP	2.0
1	A	233	GLU	2.0
1	B	65	GLY	2.0
1	B	43	VAL	2.0
1	B	152	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	TRP	A	507	15/15	0.28	1.66	53,53,53,53	0
5	FLE	A	504	15/16	0.20	0.49	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	A	501	14/15	0.20	0.39	42,45,52,61	0
3	CA	A	1	1/1	0.15	0.07	19,19,19,19	0
5	FLE	A	506	15/16	0.16	-0.80	42,42,42,42	0
3	CA	A	2	1/1	0.13	-0.82	26,26,26,26	0
4	ZN	A	503	1/1	0.20	-0.99	33,33,33,33	0
5	TRP	A	505	15/15	0.14	-1.09	16,16,16,16	0
3	CA	B	422	1/1	0.09	-1.78	24,24,24,24	0
3	CA	A	502	1/1	0.06	-1.83	34,34,34,34	0
3	CA	B	424	1/1	0.14	-3.29	72,72,72,72	0
4	ZN	B	1	1/1	0.11	-3.75	48,48,48,48	0
3	CA	B	423	1/1	0.04	-3.94	34,34,34,34	0

6.5 Other polymers ⓘ

There are no such residues in this entry.