



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 01:17 am BST

PDB ID : 1WCS
Title : A mutant of Trypanosoma rangeli sialidase displaying trans-sialidase activity
Authors : Paris, G.; Ratier, L.; Amaya, M.F.; Nguyen, T.; Alzari, P.M.; Frasch, C.
Deposited on : 2004-11-21
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

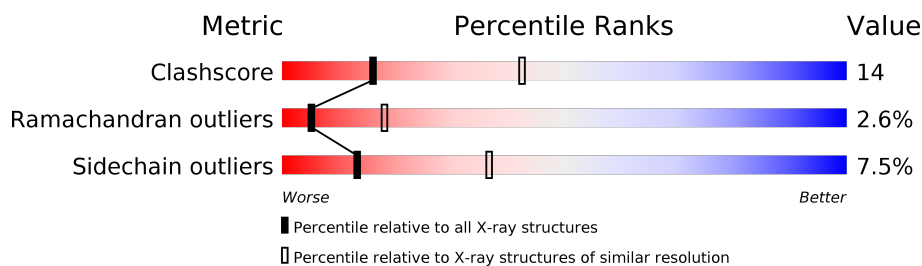
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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 on 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	641	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4841 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 SIALIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	628	Total	C	N	O	S	0	0	0
			4841	3061	850	915	15			

There are 11 discrepancies between the modelled and reference sequences:

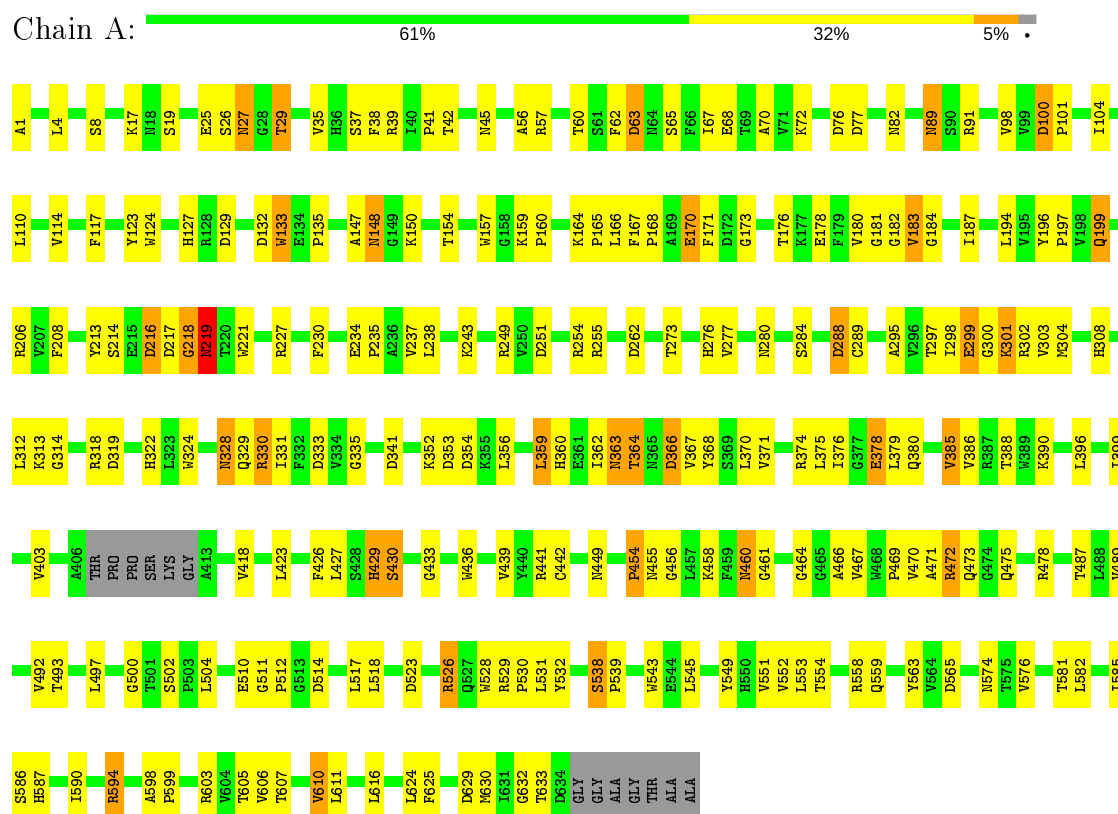
Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ILE	THR	conflict	UNP O44049
A	99	VAL	MET	engineered mutation	UNP O44049
A	101	PRO	ALA	engineered mutation	UNP O44049
A	123	TYR	SER	engineered mutation	UNP O44049
A	180	VAL	ILE	conflict	UNP O44049
A	189	ALA	ILE	conflict	UNP O44049
A	252	TYR	GLY	engineered mutation	UNP O44049
A	287	PRO	GLN	engineered mutation	UNP O44049
A	375	LEU	PHE	conflict	UNP O44049
A	413	ALA	GLY	conflict	UNP O44049
A	609	VAL	ILE	conflict	UNP O44049

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 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: SIALIDASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	94.69 Å 94.69 Å 156.34 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	158.11 – 2.80	Depositor
% Data completeness (in resolution range)	97.6 (158.11-2.80)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.244 , 0.336	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4841	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

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	0.77	9/4951 (0.2%)	0.86	17/6737 (0.3%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	299	GLU	CG-CD	17.53	1.78	1.51
1	A	299	GLU	CD-OE2	16.33	1.43	1.25
1	A	301	LYS	CE-NZ	13.38	1.82	1.49
1	A	300	GLY	C-O	11.24	1.41	1.23
1	A	329	GLN	CG-CD	10.03	1.74	1.51
1	A	300	GLY	C-N	9.95	1.56	1.34
1	A	526	ARG	CZ-NH1	7.50	1.42	1.33
1	A	299	GLU	CD-OE1	6.40	1.32	1.25
1	A	632	GLY	C-O	5.17	1.31	1.23

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	ASP	CB-CG-OD2	9.01	126.41	118.30
1	A	100	ASP	CB-CG-OD2	8.16	125.64	118.30
1	A	526	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	A	353	ASP	CB-CG-OD2	6.61	124.25	118.30
1	A	262	ASP	CB-CG-OD2	6.54	124.19	118.30
1	A	366	ASP	CB-CG-OD2	6.30	123.97	118.30
1	A	132	ASP	CB-CG-OD2	6.21	123.89	118.30
1	A	514	ASP	CB-CG-OD2	5.94	123.65	118.30
1	A	300	GLY	O-C-N	5.82	132.01	122.70
1	A	251	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	129	ASP	CB-CG-OD2	5.72	123.44	118.30
1	A	354	ASP	CB-CG-OD2	5.44	123.19	118.30
1	A	39	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	A	319	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	288	ASP	CB-CG-OD2	5.34	123.11	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	301	LYS	CD-CE-NZ	-5.03	100.13	111.70

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	4841	0	4759	139	0
All	All	4841	0	4759	139	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 14.

All (139) 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:299:GLU:CG	1:A:299:GLU:CD	1.78	1.51
1:A:301:LYS:CE	1:A:301:LYS:NZ	1.82	1.41
1:A:249:ARG:HG3	1:A:288:ASP:HB3	1.52	0.91
1:A:133:TRP:CZ2	1:A:135:PRO:HG3	2.13	0.84
1:A:1:ALA:HB3	1:A:335:GLY:HA3	1.66	0.76
1:A:289:CYS:SG	1:A:318:ARG:HD3	2.26	0.76
1:A:363:ASN:HB2	1:A:368:TYR:CE2	2.25	0.72
1:A:238:LEU:HD11	1:A:304:MET:SD	2.28	0.72
1:A:330:ARG:HB3	1:A:442:CYS:SG	2.31	0.71
1:A:299:GLU:HB3	1:A:390:LYS:HE2	1.75	0.68
1:A:523:ASP:HB3	1:A:529:ARG:HE	1.58	0.68
1:A:517:LEU:HD22	1:A:585:ILE:HD11	1.75	0.67
1:A:297:THR:OG1	1:A:302:ARG:NH1	2.27	0.67
1:A:552:VAL:HB	1:A:563:TYR:HB2	1.78	0.66
1:A:37:SER:HB3	1:A:368:TYR:HB2	1.77	0.66
1:A:466:ALA:HB3	1:A:590:ILE:HB	1.78	0.65
1:A:127:HIS:HD2	1:A:178:GLU:OE2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LYS:HA	1:A:82:ASN:O	1.97	0.63
1:A:27:ASN:HD22	1:A:27:ASN:H	1.46	0.63
1:A:299:GLU:CB	1:A:299:GLU:CD	2.66	0.62
1:A:467:VAL:O	1:A:469:PRO:HD3	1.99	0.62
1:A:301:LYS:CD	1:A:301:LYS:NZ	2.59	0.62
1:A:25:GLU:HB2	1:A:29:THR:HG23	1.82	0.61
1:A:148:ASN:HD22	1:A:148:ASN:H	1.49	0.60
1:A:301:LYS:HG3	1:A:301:LYS:NZ	2.16	0.60
1:A:388:THR:OG1	1:A:441:ARG:NH2	2.35	0.60
1:A:182:GLY:O	1:A:183:VAL:HB	2.02	0.58
1:A:295:ALA:CB	1:A:302:ARG:HH21	2.16	0.58
1:A:526:ARG:HA	1:A:543:TRP:CZ2	2.39	0.57
1:A:127:HIS:CD2	1:A:178:GLU:OE2	2.58	0.57
1:A:489:VAL:HG22	1:A:552:VAL:HG22	1.85	0.57
1:A:396:LEU:HA	1:A:399:ILE:HD12	1.87	0.57
1:A:530:PRO:HB2	1:A:532:TYR:CE1	2.40	0.56
1:A:461:GLY:H	1:A:603:ARG:HH21	1.53	0.56
1:A:594:ARG:CZ	1:A:599:PRO:HA	2.36	0.56
1:A:124:TRP:HA	1:A:127:HIS:CE1	2.41	0.55
1:A:299:GLU:HB2	1:A:386:VAL:HG11	1.88	0.55
1:A:197:PRO:HB2	1:A:235:PRO:HG2	1.88	0.55
1:A:559:GLN:HA	1:A:574:ASN:O	2.07	0.55
1:A:549:TYR:HD2	1:A:565:ASP:OD2	1.90	0.55
1:A:363:ASN:HD21	1:A:366:ASP:H	1.56	0.54
1:A:89:ASN:HD21	1:A:91:ARG:HD3	1.73	0.54
1:A:473:GLN:OE1	1:A:478:ARG:HB2	2.07	0.54
1:A:289:CYS:HB2	1:A:318:ARG:HE	1.73	0.54
1:A:385:VAL:HA	1:A:441:ARG:NH2	2.23	0.53
1:A:518:LEU:HG	1:A:553:LEU:HD22	1.91	0.53
1:A:217:ASP:C	1:A:219:ASN:H	2.11	0.53
1:A:295:ALA:HB1	1:A:302:ARG:HH21	1.73	0.53
1:A:194:LEU:O	1:A:213:TYR:HA	2.09	0.53
1:A:217:ASP:O	1:A:219:ASN:N	2.41	0.52
1:A:62:PHE:O	1:A:65:SER:OG	2.14	0.52
1:A:427:LEU:HB3	1:A:436:TRP:CE2	2.45	0.52
1:A:470:VAL:HG23	1:A:587:HIS:HA	1.92	0.52
1:A:57:ARG:HG2	1:A:67:ILE:HG12	1.91	0.51
1:A:101:PRO:HA	1:A:114:VAL:HG12	1.91	0.51
1:A:312:LEU:O	1:A:314:GLY:N	2.44	0.51
1:A:471:ALA:C	1:A:473:GLN:H	2.14	0.51
1:A:45:ASN:HB2	1:A:352:LYS:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ASP:N	1:A:101:PRO:HD3	2.25	0.51
1:A:187:ILE:HG21	1:A:238:LEU:HA	1.91	0.51
1:A:558:ARG:O	1:A:576:VAL:HG22	2.10	0.51
1:A:399:ILE:HD13	1:A:630:MET:O	2.10	0.51
1:A:77:ASP:OD2	1:A:352:LYS:NZ	2.44	0.51
1:A:487:THR:HG23	1:A:554:THR:HG22	1.93	0.50
1:A:526:ARG:HA	1:A:543:TRP:CE2	2.46	0.50
1:A:35:VAL:HB	1:A:38:PHE:CZ	2.45	0.50
1:A:255:ARG:HH21	1:A:308:HIS:HE1	1.60	0.49
1:A:124:TRP:HA	1:A:127:HIS:NE2	2.28	0.49
1:A:359:LEU:HD23	1:A:371:VAL:O	2.12	0.49
1:A:551:VAL:HA	1:A:563:TYR:O	2.12	0.49
1:A:375:LEU:HB3	1:A:378:GLU:HB2	1.95	0.49
1:A:454:PRO:O	1:A:455:ASN:HB2	2.13	0.49
1:A:493:THR:OG1	1:A:605:THR:HB	2.12	0.49
1:A:492:VAL:HG12	1:A:606:VAL:HG22	1.95	0.48
1:A:610:VAL:HG12	1:A:611:LEU:H	1.77	0.48
1:A:528:TRP:CZ2	1:A:543:TRP:HB3	2.48	0.48
1:A:487:THR:HG21	1:A:616:LEU:HD12	1.95	0.48
1:A:363:ASN:HD21	1:A:366:ASP:N	2.11	0.48
1:A:68:GLU:HA	1:A:98:VAL:CG2	2.44	0.48
1:A:68:GLU:HA	1:A:98:VAL:HG22	1.96	0.48
1:A:487:THR:HA	1:A:553:LEU:O	2.13	0.48
1:A:104:ILE:HG13	1:A:196:TYR:CE2	2.49	0.48
1:A:8:SER:HB3	1:A:374:ARG:O	2.14	0.48
1:A:199:GLN:NE2	1:A:234:GLU:H	2.12	0.47
1:A:301:LYS:NZ	1:A:301:LYS:CG	2.77	0.47
1:A:110:LEU:HD13	1:A:157:TRP:CH2	2.49	0.47
1:A:41:PRO:HG3	1:A:360:HIS:HA	1.96	0.47
1:A:133:TRP:HZ2	1:A:135:PRO:HG3	1.70	0.47
1:A:56:ALA:HB2	1:A:70:ALA:HB2	1.97	0.47
1:A:148:ASN:H	1:A:148:ASN:ND2	2.12	0.47
1:A:363:ASN:HD22	1:A:364:THR:N	2.13	0.47
1:A:17:LYS:HE3	1:A:367:VAL:HG11	1.97	0.46
1:A:363:ASN:HB2	1:A:368:TYR:CD2	2.50	0.46
1:A:4:LEU:HD12	1:A:378:GLU:OE2	2.16	0.46
1:A:216:ASP:CG	1:A:219:ASN:HB3	2.35	0.46
1:A:362:ILE:HG13	1:A:362:ILE:O	2.15	0.46
1:A:171:PHE:CD1	1:A:176:THR:HG21	2.51	0.46
1:A:472:ARG:HD2	1:A:586:SER:HB2	1.98	0.46
1:A:180:VAL:HG12	1:A:181:GLY:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:THR:OG1	1:A:184:GLY:HA2	2.16	0.45
1:A:458:LYS:HE2	1:A:460:ASN:HD22	1.81	0.45
1:A:167:PHE:CE2	1:A:176:THR:HB	2.52	0.45
1:A:426:PHE:HB3	1:A:439:VAL:HB	1.99	0.45
1:A:170:GLU:HG2	1:A:173:GLY:H	1.81	0.45
1:A:418:VAL:HG13	1:A:624:LEU:HD23	1.99	0.45
1:A:41:PRO:HB3	1:A:370:LEU:HD22	1.99	0.44
1:A:429:HIS:O	1:A:430:SER:C	2.56	0.44
1:A:148:ASN:HD22	1:A:148:ASN:N	2.08	0.44
1:A:159:LYS:HA	1:A:160:PRO:HD3	1.87	0.44
1:A:166:LEU:O	1:A:168:PRO:HD3	2.18	0.44
1:A:449:ASN:HB2	1:A:464:GLY:HA3	2.00	0.43
1:A:164:LYS:N	1:A:165:PRO:CD	2.81	0.43
1:A:363:ASN:ND2	1:A:363:ASN:C	2.72	0.43
1:A:324:TRP:CD1	1:A:333:ASP:HA	2.54	0.42
1:A:322:HIS:HB2	1:A:324:TRP:CZ3	2.54	0.42
1:A:117:PHE:CE2	1:A:133:TRP:HB2	2.53	0.42
1:A:218:GLY:HA2	1:A:221:TRP:CZ2	2.54	0.42
1:A:456:GLY:HA3	1:A:607:THR:HG22	2.00	0.42
1:A:206:ARG:HB3	1:A:230:PHE:CD2	2.54	0.42
1:A:461:GLY:N	1:A:603:ARG:HH21	2.15	0.42
1:A:328:ASN:HA	1:A:328:ASN:HD22	1.62	0.42
1:A:497:LEU:HG	1:A:545:LEU:HD11	2.01	0.42
1:A:208:PHE:CE1	1:A:227:ARG:HD2	2.55	0.42
1:A:511:GLY:HA3	1:A:512:PRO:HD3	1.80	0.42
1:A:538:SER:HA	1:A:539:PRO:HD3	1.90	0.42
1:A:418:VAL:HG13	1:A:624:LEU:CD2	2.50	0.42
1:A:254:ARG:HB2	1:A:276:HIS:ND1	2.35	0.41
1:A:277:VAL:HG11	1:A:331:ILE:HD13	2.02	0.41
1:A:104:ILE:HG21	1:A:194:LEU:HD22	2.02	0.41
1:A:214:SER:OG	1:A:216:ASP:OD2	2.38	0.41
1:A:492:VAL:HG11	1:A:504:LEU:HD21	2.02	0.41
1:A:385:VAL:HG22	1:A:441:ARG:NH1	2.35	0.41
1:A:510:GLU:HG2	1:A:586:SER:HB3	2.03	0.41
1:A:363:ASN:ND2	1:A:366:ASP:HA	2.36	0.40
1:A:598:ALA:HA	1:A:599:PRO:HD3	1.93	0.40
1:A:298:ILE:HG22	1:A:386:VAL:HG21	2.03	0.40
1:A:63:ASP:HB2	1:A:123:TYR:HE2	1.86	0.40
1:A:331:ILE:O	1:A:478:ARG:HD3	2.21	0.40
1:A:356:LEU:HB2	1:A:379:LEU:HD13	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	624/641 (97%)	531 (85%)	77 (12%)	16 (3%)	5	18

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	SER
1	A	313	LYS
1	A	475	GLN
1	A	183	VAL
1	A	403	VAL
1	A	430	SER
1	A	433	GLY
1	A	63	ASP
1	A	429	HIS
1	A	219	ASN
1	A	454	PRO
1	A	500	GLY
1	A	147	ALA
1	A	218	GLY
1	A	378	GLU
1	A	472	ARG

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	521/533 (98%)	482 (92%)	39 (8%)	13 37

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	SER
1	A	27	ASN
1	A	29	THR
1	A	60	THR
1	A	76	ASP
1	A	89	ASN
1	A	133	TRP
1	A	148	ASN
1	A	150	LYS
1	A	154	THR
1	A	170	GLU
1	A	199	GLN
1	A	219	ASN
1	A	237	VAL
1	A	243	LYS
1	A	273	THR
1	A	280	ASN
1	A	284	SER
1	A	303	VAL
1	A	328	ASN
1	A	330	ARG
1	A	359	LEU
1	A	363	ASN
1	A	364	THR
1	A	376	ILE
1	A	380	GLN
1	A	385	VAL
1	A	423	LEU
1	A	460	ASN
1	A	502	SER
1	A	531	LEU
1	A	538	SER
1	A	581	THR
1	A	582	LEU
1	A	594	ARG

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Mol	Chain	Res	Type
1	A	610	VAL
1	A	625	PHE
1	A	629	ASP
1	A	633	THR

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

Mol	Chain	Res	Type
1	A	27	ASN
1	A	89	ASN
1	A	127	HIS
1	A	148	ASN
1	A	199	GLN
1	A	253	ASN
1	A	280	ASN
1	A	328	ASN
1	A	329	GLN
1	A	336	GLN
1	A	363	ASN
1	A	460	ASN
1	A	574	ASN
1	A	608	ASN
1	A	628	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

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 ⓘ

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.