



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:38 PM UTC

PDB ID : 1WCS / pdb_00001wcs
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 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
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

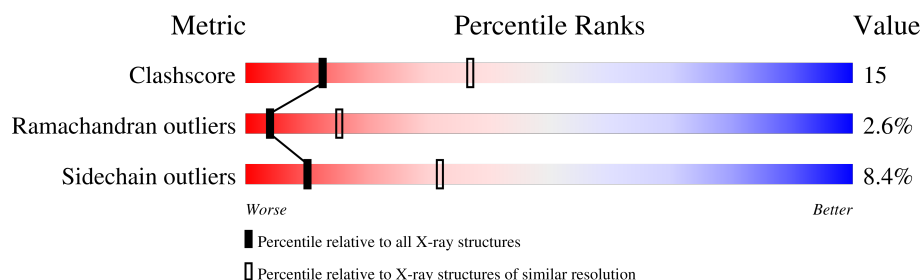
1 Overall quality at a glance

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	641	 60% 32% 5%

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
			Total	C	N	O	S			
1	A	628	4841	3061	850	915	15	0	0	0

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

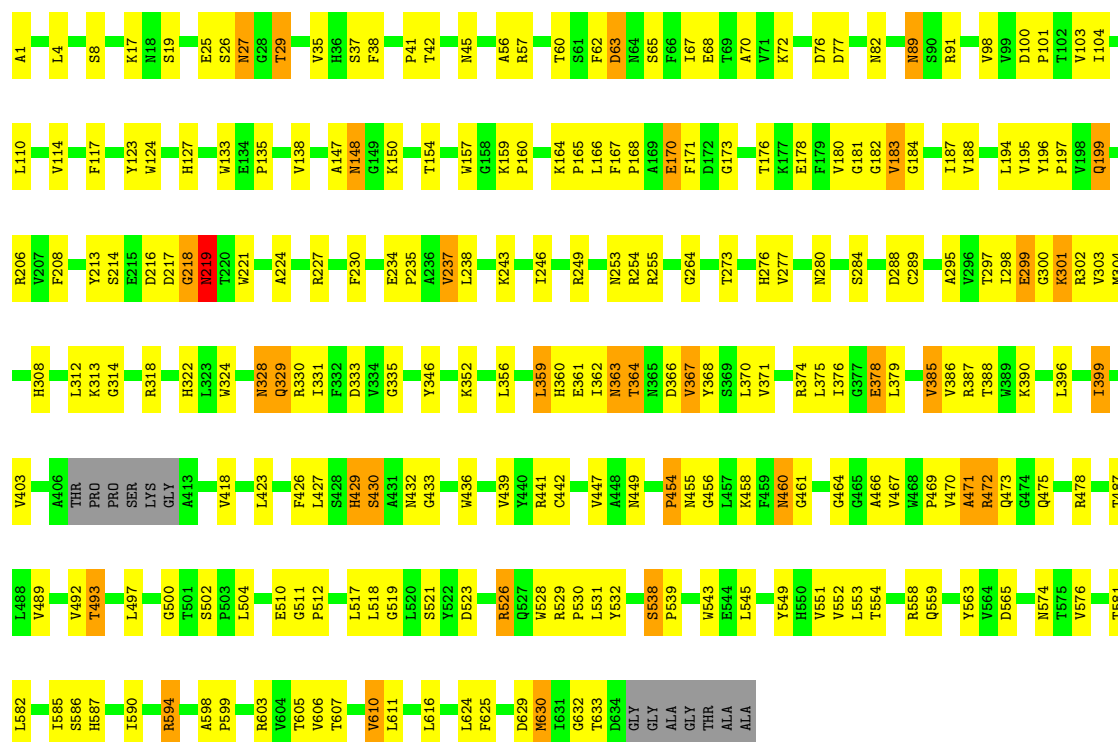
3 Residue-property plots

These plots are drawn for all protein, RNA, 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: SIALIDASE

Chain A: 



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	94.69Å 94.69Å 156.34Å 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 [i](#)

5.1 Standard geometry [i](#)

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	0.87	8/4951 (0.2%)	1.04	7/6737 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	300	GLY	C-N	17.00	1.56	1.33
1	A	300	GLY	C-O	11.81	1.41	1.24
1	A	301	LYS	CE-NZ	11.05	1.82	1.49
1	A	299	GLU	CG-CD	10.48	1.78	1.52
1	A	299	GLU	CD-OE2	9.62	1.43	1.25
1	A	329	GLN	CG-CD	8.83	1.74	1.52
1	A	632	GLY	C-O	7.77	1.31	1.23
1	A	526	ARG	CZ-NH1	7.17	1.42	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	300	GLY	O-C-N	8.75	132.01	122.56
1	A	432	ASN	N-CA-C	6.62	119.26	107.80
1	A	195	VAL	N-CA-C	5.95	116.18	106.72
1	A	471	ALA	N-CA-C	-5.85	106.28	113.41
1	A	519	GLY	N-CA-C	5.49	118.50	110.38
1	A	103	VAL	N-CA-C	5.16	115.55	108.12
1	A	237	VAL	N-CA-C	5.07	116.02	108.46

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	146	0
All	All	4841	0	4759	146	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 15.

All (146) 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:CD	1:A:299:GLU:CG	1.78	1.53
1:A:301:LYS:NZ	1:A:301:LYS:CE	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:CD	1:A:299:GLU:CB	2.66	0.69
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
1:A:72:LYS:HA	1:A:82:ASN:O	1.97	0.63
1:A:27:ASN:H	1:A:27:ASN:HD22	1.46	0.63
1:A:467:VAL:O	1:A:469:PRO:HD3	1.99	0.62
1:A:301:LYS:NZ	1:A:301:LYS:CD	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:NZ	1:A:301:LYS:HG3	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:217:ASP:C	1:A:219:ASN:H	2.11	0.57
1:A:526:ARG:HA	1:A:543:TRP:CZ2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:471:ALA:C	1:A:473:GLN:H	2.14	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: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:62:PHE:O	1:A:65:SER:OG	2.14	0.52
1:A:217:ASP:O	1:A:219:ASN:N	2.41	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:45:ASN:HB2	1:A:352:LYS:HD2	1.93	0.51
1:A:216:ASP:CG	1:A:219:ASN:HB3	2.35	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:429:HIS:O	1:A:430:SER:C	2.56	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: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:363:ASN:HD21	1:A:366:ASP:N	2.11	0.48
1:A:487:THR:HA	1:A:553:LEU:O	2.13	0.48
1:A:8:SER:HB3	1:A:374:ARG:O	2.14	0.48
1:A:104:ILE:HG13	1:A:196:TYR:CE2	2.49	0.48
1:A:363:ASN:C	1:A:363:ASN:ND2	2.72	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:41:PRO:HG3	1:A:360:HIS:HA	1.96	0.47
1:A:110:LEU:HD13	1:A:157:TRP:CH2	2.49	0.47
1:A:56:ALA:HB2	1:A:70:ALA:HB2	1.97	0.47
1:A:133:TRP:HZ2	1:A:135:PRO:HG3	1.70	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:4:LEU:HD12	1:A:378:GLU:OE2	2.16	0.46
1:A:363:ASN:HB2	1:A:368:TYR:CD2	2.50	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
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:346:TYR:HB2	1:A:361:GLU:CD	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ALA:HB1	1:A:264:GLY:C	2.43	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:328:ASN:C	1:A:329:GLN:HG3	2.42	0.43
1:A:322:HIS:HB2	1:A:324:TRP:CZ3	2.54	0.42
1:A:324:TRP:CD1	1:A:333:ASP:HA	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:HD22	1:A:328:ASN:HA	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:418:VAL:HG13	1:A:624:LEU:CD2	2.50	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:253:ASN:CG	1:A:254:ARG:H	2.28	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:387:ARG:O	1:A:388:THR:C	2.63	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:312:LEU:C	1:A:314:GLY:N	2.80	0.40
1:A:298:ILE:HG22	1:A:386:VAL:HG21	2.03	0.40
1:A:521:SER:C	1:A:529:ARG:HB2	2.47	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%)	4	15

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%)	477 (92%)	44 (8%)	10 32

All (44) 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	138	VAL
1	A	148	ASN
1	A	150	LYS
1	A	154	THR
1	A	170	GLU
1	A	188	VAL
1	A	199	GLN
1	A	219	ASN
1	A	237	VAL
1	A	243	LYS
1	A	246	ILE
1	A	273	THR
1	A	280	ASN
1	A	284	SER
1	A	303	VAL
1	A	328	ASN
1	A	359	LEU
1	A	363	ASN
1	A	364	THR
1	A	367	VAL
1	A	376	ILE
1	A	385	VAL
1	A	399	ILE
1	A	423	LEU
1	A	447	VAL
1	A	460	ASN
1	A	493	THR
1	A	502	SER
1	A	531	LEU

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Mol	Chain	Res	Type
1	A	538	SER
1	A	581	THR
1	A	582	LEU
1	A	594	ARG
1	A	610	VAL
1	A	625	PHE
1	A	629	ASP
1	A	630	MET
1	A	633	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) 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	363	ASN
1	A	460	ASN
1	A	574	ASN
1	A	608	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

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.