



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:53 PM GMT

PDB ID : 1HRH
Title : CRYSTAL STRUCTURE OF THE RIBONUCLEASE H DOMAIN OF HIV-1
REVERSE TRANSCRIPTASE
Authors : Davies /II, J.F.; Matthews, D.A.
Deposited on : 1991-03-06
Resolution : 2.40 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

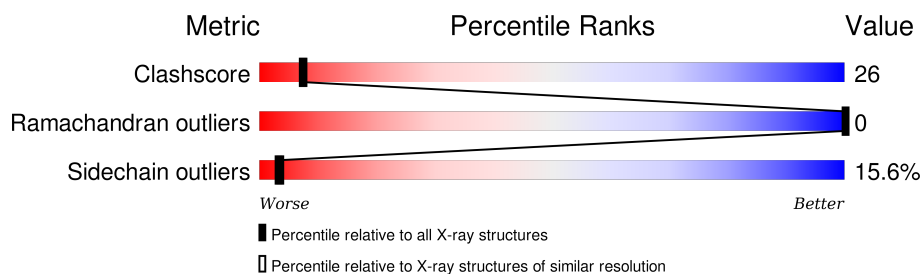
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

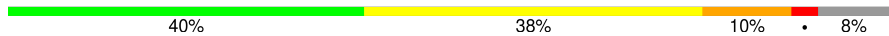
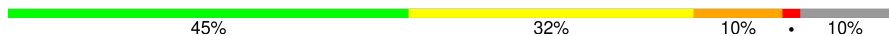
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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. 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 $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	136	
1	B	136	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1803 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 RIBONUCLEASE H.

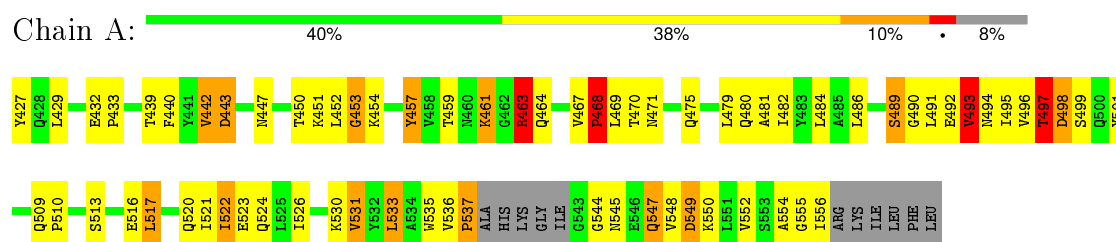
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	125	Total	C	N	O	0	0	0
			921	587	151	183			
1	B	122	Total	C	N	O	0	0	0
			882	561	147	174			

3 Residue-property plots

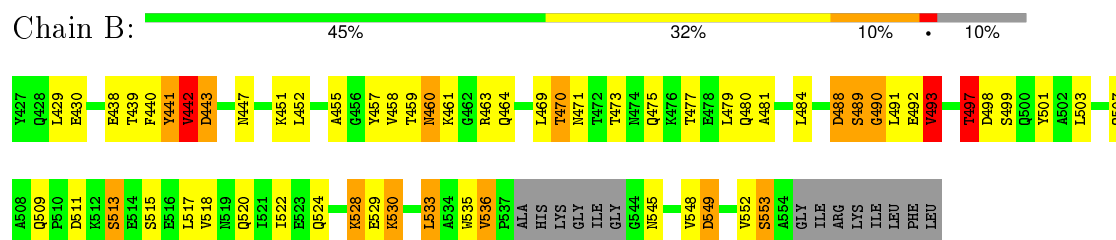
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: RIBONUCLEASE H



• Molecule 1: RIBONUCLEASE H



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	51.90Å 51.90Å 114.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.200 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1803	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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	1.22	2/932 (0.2%)	2.08	25/1270 (2.0%)
1	B	1.25	2/893 (0.2%)	2.16	33/1222 (2.7%)
All	All	1.23	4/1825 (0.2%)	2.12	58/2492 (2.3%)

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	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	490	GLY	N-CA	10.27	1.61	1.46
1	A	490	GLY	N-CA	9.30	1.59	1.46
1	A	489	SER	CB-OG	6.04	1.50	1.42
1	B	489	SER	C-O	6.02	1.34	1.23

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	498	ASP	CB-CG-OD1	11.69	128.82	118.30
1	A	463	ARG	NE-CZ-NH2	-11.27	114.66	120.30
1	A	463	ARG	NE-CZ-NH1	10.39	125.49	120.30
1	B	501	TYR	CB-CG-CD2	10.28	127.17	121.00
1	B	501	TYR	CB-CG-CD1	-9.94	115.04	121.00
1	A	464	GLN	N-CA-CB	9.56	127.82	110.60
1	B	489	SER	N-CA-C	8.66	134.38	111.00
1	B	442	VAL	CG1-CB-CG2	8.35	124.25	110.90
1	B	463	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	B	442	VAL	N-CA-CB	-8.13	93.61	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	489	SER	CA-C-N	8.05	132.31	116.20
1	B	493	VAL	CB-CA-C	-7.57	97.02	111.40
1	A	549	ASP	CB-CG-OD1	7.52	125.07	118.30
1	A	497	THR	CA-CB-CG2	7.36	122.70	112.40
1	B	545	ASN	CB-CA-C	7.25	124.89	110.40
1	A	497	THR	CB-CA-C	-6.82	93.18	111.60
1	A	489	SER	CA-C-N	6.78	129.76	116.20
1	A	489	SER	C-N-CA	-6.77	108.08	122.30
1	B	479	LEU	CA-C-O	6.76	134.29	120.10
1	B	475	GLN	CB-CG-CD	6.65	128.89	111.60
1	A	498	ASP	CB-CG-OD2	-6.54	112.42	118.30
1	B	438	GLU	OE1-CD-OE2	6.39	130.97	123.30
1	B	479	LEU	CA-CB-CG	6.38	129.96	115.30
1	B	455	ALA	C-N-CA	-6.30	109.07	122.30
1	B	497	THR	CB-CA-C	-6.24	94.76	111.60
1	B	530	LYS	O-C-N	6.19	132.60	122.70
1	B	489	SER	C-N-CA	-6.17	109.35	122.30
1	A	493	VAL	CB-CA-C	-6.14	99.73	111.40
1	B	528	LYS	CA-CB-CG	6.03	126.67	113.40
1	B	533	LEU	CA-C-O	-6.02	107.45	120.10
1	B	549	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	B	497	THR	O-C-N	5.86	132.08	122.70
1	B	515	SER	N-CA-CB	5.81	119.21	110.50
1	A	453	GLY	C-N-CA	5.80	136.21	121.70
1	B	443	ASP	CB-CG-OD1	5.72	123.45	118.30
1	B	441	TYR	CA-C-O	5.72	132.10	120.10
1	A	475	GLN	CB-CG-CD	5.69	126.39	111.60
1	A	464	GLN	CB-CA-C	-5.66	99.09	110.40
1	A	443	ASP	CB-CG-OD1	5.55	123.29	118.30
1	A	552	VAL	N-CA-CB	-5.50	99.39	111.50
1	B	513	SER	O-C-N	-5.50	113.90	122.70
1	A	497	THR	CA-C-N	-5.48	105.15	117.20
1	B	479	LEU	O-C-N	-5.46	113.97	122.70
1	A	468	PRO	CB-CA-C	5.38	125.46	112.00
1	A	457	TYR	CB-CG-CD2	5.31	124.19	121.00
1	A	501	TYR	CZ-CE2-CD2	-5.29	115.04	119.80
1	B	430	GLU	CG-CD-OE1	5.29	128.88	118.30
1	A	549	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	A	442	VAL	N-CA-CB	-5.25	99.96	111.50
1	B	530	LYS	CA-C-N	-5.20	105.77	117.20
1	A	552	VAL	CB-CA-C	5.18	121.24	111.40
1	B	490	GLY	N-CA-C	-5.17	100.17	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	489	SER	O-C-N	-5.16	114.44	123.20
1	B	464	GLN	N-CA-CB	-5.08	101.46	110.60
1	A	497	THR	O-C-N	5.06	130.80	122.70
1	B	530	LYS	N-CA-CB	5.04	119.68	110.60
1	B	460	ASN	CB-CG-OD1	-5.01	111.57	121.60
1	B	511	ASP	N-CA-C	-5.01	97.47	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	463	ARG	Sidechain

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	921	0	901	55	0
1	B	882	0	838	36	0
All	All	1803	0	1739	91	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 26.

All (91) 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:495:ILE:HB	1:A:533:LEU:HD23	1.48	0.95
1:A:520:GLN:O	1:A:523:GLU:HG2	1.71	0.89
1:A:463:ARG:HH11	1:A:463:ARG:HB2	1.46	0.81
1:A:469:LEU:HD11	1:A:480:GLN:HG2	1.65	0.78
1:B:457:TYR:O	1:B:458:VAL:HG23	1.83	0.78
1:B:492:GLU:HA	1:B:530:LYS:O	1.86	0.75
1:A:498:ASP:HA	1:A:536:VAL:O	1.88	0.74
1:B:535:TRP:O	1:B:536:VAL:HG23	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:GLN:N	1:A:510:PRO:HD3	2.06	0.71
1:A:454:LYS:NZ	1:A:554:ALA:O	2.25	0.69
1:A:440:PHE:CD2	1:A:459:THR:HG22	2.29	0.67
1:A:432:GLU:HB3	1:A:433:PRO:HD2	1.77	0.67
1:B:498:ASP:HA	1:B:536:VAL:O	1.99	0.62
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.02	0.59
1:B:460:ASN:C	1:B:460:ASN:OD1	2.38	0.59
1:A:516:GLU:O	1:A:520:GLN:HG3	2.03	0.58
1:A:427:TYR:OH	1:A:509:GLN:HA	2.03	0.58
1:B:497:THR:HB	1:B:499:SER:H	1.69	0.57
1:A:493:VAL:HG23	1:A:531:VAL:HB	1.87	0.56
1:A:439:THR:HA	1:A:494:ASN:HB2	1.89	0.55
1:A:497:THR:HB	1:A:499:SER:H	1.72	0.55
1:A:545:ASN:HA	1:A:548:VAL:HG12	1.88	0.55
1:A:479:LEU:O	1:A:521:ILE:HD11	2.07	0.55
1:A:495:ILE:HB	1:A:533:LEU:CD2	2.30	0.55
1:B:470:THR:CG2	1:B:470:THR:O	2.55	0.54
1:A:489:SER:HB2	1:A:493:VAL:HG13	1.89	0.54
1:A:457:TYR:CD1	1:A:457:TYR:C	2.80	0.54
1:B:457:TYR:OH	1:B:488:ASP:OD2	2.26	0.53
1:B:460:ASN:OD1	1:B:461:LYS:N	2.42	0.53
1:B:470:THR:HG23	1:B:470:THR:O	2.09	0.52
1:B:549:ASP:O	1:B:553:SER:OG	2.26	0.52
1:A:427:TYR:HE2	1:A:429:LEU:HD11	1.74	0.52
1:B:440:PHE:CD2	1:B:459:THR:HG22	2.45	0.52
1:A:461:LYS:NZ	1:A:461:LYS:HA	2.25	0.52
1:A:522:ILE:O	1:A:526:ILE:HG13	2.10	0.52
1:A:463:ARG:NH1	1:A:463:ARG:HB2	2.20	0.52
1:A:509:GLN:N	1:A:510:PRO:CD	2.72	0.51
1:B:524:GLN:HA	1:B:524:GLN:OE1	2.10	0.51
1:B:443:ASP:HB2	1:B:548:VAL:HG13	1.92	0.51
1:B:503:LEU:O	1:B:507:GLN:HG3	2.11	0.51
1:B:439:THR:O	1:B:459:THR:HA	2.11	0.50
1:B:491:LEU:O	1:B:529:GLU:N	2.44	0.50
1:A:461:LYS:HA	1:A:461:LYS:HZ1	1.78	0.49
1:A:486:LEU:HD13	1:A:524:GLN:HB2	1.94	0.49
1:A:440:PHE:CG	1:A:459:THR:HG22	2.48	0.48
1:B:518:VAL:O	1:B:522:ILE:HG13	2.14	0.47
1:B:517:LEU:O	1:B:520:GLN:HB2	2.14	0.47
1:A:535:TRP:CH2	1:A:537:PRO:HB3	2.49	0.47
1:A:517:LEU:HA	1:A:517:LEU:HD23	1.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:LEU:HD11	1:B:480:GLN:HG2	1.96	0.47
1:B:497:THR:O	1:B:535:TRP:HA	2.15	0.47
1:A:467:VAL:HG13	1:A:468:PRO:HD2	1.97	0.46
1:B:451:LYS:O	1:B:471:ASN:HA	2.15	0.46
1:A:537:PRO:O	1:A:537:PRO:HG2	2.15	0.46
1:A:549:ASP:O	1:A:550:LYS:C	2.54	0.46
1:B:442:VAL:HG13	1:B:481:ALA:HB1	1.98	0.46
1:A:440:PHE:CE2	1:A:459:THR:CG2	2.99	0.46
1:B:489:SER:HB2	1:B:493:VAL:HG13	1.97	0.45
1:B:473:THR:O	1:B:477:THR:HG23	2.16	0.45
1:A:489:SER:CB	1:A:493:VAL:HG13	2.46	0.45
1:B:440:PHE:CE2	1:B:459:THR:HG21	2.51	0.45
1:B:470:THR:O	1:B:471:ASN:C	2.54	0.45
1:B:451:LYS:O	1:B:471:ASN:CA	2.65	0.45
1:A:482:ILE:HD11	1:A:497:THR:HG21	1.99	0.45
1:A:440:PHE:CZ	1:A:459:THR:HG21	2.52	0.45
1:A:470:THR:O	1:A:471:ASN:CB	2.63	0.45
1:A:454:LYS:HA	1:A:467:VAL:O	2.16	0.44
1:B:490:GLY:O	1:B:528:LYS:NZ	2.49	0.44
1:A:492:GLU:HA	1:A:530:LYS:O	2.18	0.44
1:A:432:GLU:HB3	1:A:433:PRO:CD	2.46	0.44
1:B:535:TRP:O	1:B:536:VAL:CG2	2.64	0.43
1:B:447:ASN:O	1:B:451:LYS:HA	2.18	0.43
1:B:441:TYR:O	1:B:548:VAL:HG11	2.19	0.43
1:B:469:LEU:HD11	1:B:480:GLN:CG	2.48	0.43
1:B:457:TYR:HA	1:B:548:VAL:HG21	2.01	0.43
1:B:469:LEU:HD23	1:B:469:LEU:HA	1.66	0.43
1:A:453:GLY:O	1:A:469:LEU:N	2.42	0.43
1:A:555:GLY:O	1:A:556:ILE:HG13	2.18	0.42
1:A:450:THR:CB	1:A:452:LEU:HG	2.50	0.42
1:A:544:GLY:HA2	1:A:547:GLN:NE2	2.35	0.41
1:A:497:THR:O	1:A:535:TRP:HA	2.20	0.41
1:A:443:ASP:O	1:A:481:ALA:HB2	2.20	0.41
1:A:491:LEU:HD23	1:A:491:LEU:HA	1.91	0.41
1:A:467:VAL:HA	1:A:468:PRO:HD3	1.83	0.41
1:B:451:LYS:O	1:B:471:ASN:N	2.53	0.41
1:A:492:GLU:HG2	1:A:530:LYS:HB2	2.01	0.41
1:A:523:GLU:HG2	1:A:524:GLN:N	2.36	0.41
1:A:447:ASN:O	1:A:451:LYS:N	2.45	0.41
1:A:523:GLU:CG	1:A:524:GLN:N	2.84	0.40
1:A:496:VAL:CG2	1:A:496:VAL:O	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:ILE:HD11	1:A:497:THR:CG2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	121/136 (89%)	113 (93%)	8 (7%)	0	100	100
1	B	118/136 (87%)	109 (92%)	9 (8%)	0	100	100
All	All	239/272 (88%)	222 (93%)	17 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	93/114 (82%)	79 (85%)	14 (15%)	3	4
1	B	86/114 (75%)	72 (84%)	14 (16%)	3	3
All	All	179/228 (78%)	151 (84%)	28 (16%)	3	3

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	442	VAL
1	A	461	LYS
1	A	463	ARG
1	A	468	PRO
1	A	484	LEU
1	A	493	VAL
1	A	497	THR
1	A	513	SER
1	A	517	LEU
1	A	522	ILE
1	A	531	VAL
1	A	533	LEU
1	A	537	PRO
1	A	547	GLN
1	B	429	LEU
1	B	442	VAL
1	B	452	LEU
1	B	470	THR
1	B	484	LEU
1	B	488	ASP
1	B	493	VAL
1	B	497	THR
1	B	509	GLN
1	B	513	SER
1	B	533	LEU
1	B	536	VAL
1	B	552	VAL
1	B	553	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	520	GLN
1	A	547	GLN
1	B	480	GLN
1	B	507	GLN

5.3.3 RNA ⓘ

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 [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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.