



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:13 PM UTC

PDB ID : 1HRH / pdb_00001hrh
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

<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

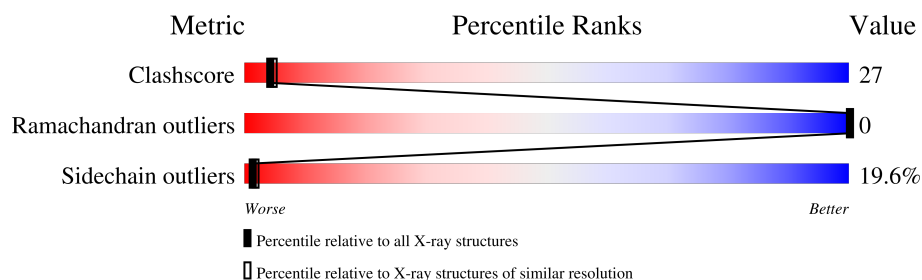
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

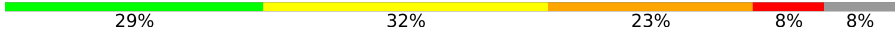
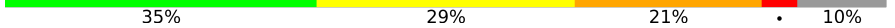
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (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 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	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.

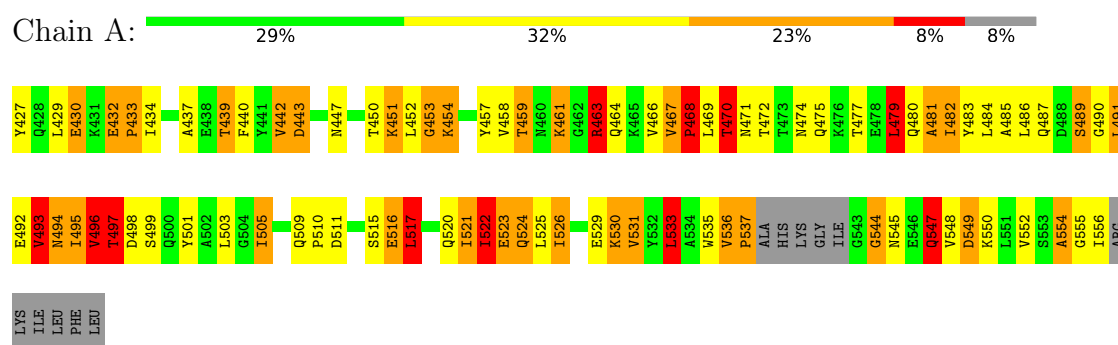
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	125	Total	C	N	O	0	0	0
			921	587	151	183			
1	B	122	Total	C	N	O	0	0	0
			882	561	147	174			

3 Residue-property plots

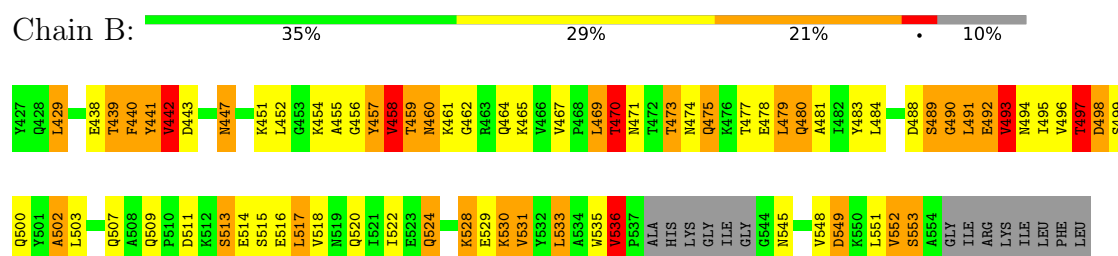
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: RIBONUCLEASE H



• Molecule 1: RIBONUCLEASE H



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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	1.61	6/932 (0.6%)	2.71	91/1270 (7.2%)
1	B	1.68	9/893 (1.0%)	2.79	84/1222 (6.9%)
All	All	1.64	15/1825 (0.8%)	2.75	175/2492 (7.0%)

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 (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	490	GLY	N-CA	11.09	1.61	1.45
1	A	490	GLY	N-CA	10.09	1.59	1.45
1	B	489	SER	C-O	8.40	1.34	1.24
1	B	470	THR	CA-CB	7.11	1.64	1.53
1	B	479	LEU	N-CA	6.02	1.53	1.46
1	B	439	THR	CA-CB	5.99	1.62	1.53
1	B	495	ILE	N-CA	5.96	1.53	1.46
1	A	489	SER	C-O	5.69	1.32	1.23
1	B	497	THR	CA-CB	5.62	1.62	1.53
1	B	483	TYR	N-CA	5.62	1.53	1.46
1	A	505	ILE	C-O	-5.49	1.18	1.24
1	A	485	ALA	C-O	-5.44	1.17	1.24
1	B	456	GLY	N-CA	5.39	1.53	1.45
1	A	470	THR	CA-CB	5.29	1.60	1.53
1	A	495	ILE	N-CA	5.20	1.52	1.46

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	489	SER	N-CA-C	15.78	134.38	112.45
1	B	479	LEU	CA-C-O	13.09	134.29	120.42
1	B	533	LEU	CA-C-O	-12.27	107.45	120.70
1	B	429	LEU	CA-C-O	-10.44	109.64	120.71
1	A	432	GLU	O-C-N	10.18	128.22	121.71
1	B	464	GLN	OE1-CD-NE2	9.94	132.54	122.60
1	A	464	GLN	N-CA-CB	9.68	127.82	111.66
1	A	497	THR	CB-CA-C	-9.65	93.18	110.36
1	B	442	VAL	N-CA-CB	-9.65	93.61	110.49
1	B	475	GLN	CB-CG-CD	9.58	128.89	112.60
1	B	441	TYR	CA-C-O	9.56	132.10	121.39
1	A	533	LEU	CA-C-O	-9.44	110.20	120.30
1	B	480	GLN	CA-C-N	9.28	133.69	120.79
1	B	480	GLN	C-N-CA	9.28	133.69	120.79
1	B	514	GLU	N-CA-C	-9.19	101.59	113.17
1	A	463	ARG	CA-C-O	-9.08	110.70	121.05
1	A	487	GLN	CA-C-O	-8.93	110.95	120.42
1	A	479	LEU	CA-C-O	8.93	130.36	119.38
1	B	500	GLN	OE1-CD-NE2	-8.82	113.78	122.60
1	A	505	ILE	N-CA-C	-8.74	102.20	110.42
1	B	551	LEU	N-CA-C	8.65	120.71	111.28
1	B	494	ASN	CA-C-O	-8.63	110.74	120.32
1	A	453	GLY	CA-C-N	8.54	136.21	122.81
1	A	453	GLY	C-N-CA	8.54	136.21	122.81
1	A	536	VAL	N-CA-C	-8.54	102.19	109.19
1	A	437	ALA	CA-C-N	8.51	133.59	121.42
1	A	437	ALA	C-N-CA	8.51	133.59	121.42
1	A	468	PRO	CB-CA-C	8.42	125.46	111.56
1	B	497	THR	CB-CA-C	-8.31	94.76	109.71
1	A	430	GLU	CA-C-O	-8.25	113.35	122.01
1	A	515	SER	CA-C-O	8.18	129.29	120.38
1	A	475	GLN	CB-CG-CD	8.11	126.39	112.60
1	A	522	ILE	O-C-N	8.11	129.73	121.87
1	B	549	ASP	CA-CB-CG	-8.10	104.50	112.60
1	B	493	VAL	CB-CA-C	-7.86	97.02	110.30
1	B	470	THR	N-CA-C	7.76	121.56	109.07
1	A	544	GLY	N-CA-C	-7.67	103.08	113.37
1	A	501	TYR	O-C-N	7.58	129.88	122.07
1	B	530	LYS	O-C-N	7.45	132.60	123.44
1	A	525	LEU	O-C-N	7.22	129.78	122.12
1	A	511	ASP	O-C-N	7.21	130.61	122.32
1	B	513	SER	O-C-N	-7.19	113.90	122.96
1	A	497	THR	CA-CB-CG2	7.18	122.70	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	479	LEU	O-C-N	-7.17	113.97	122.15
1	B	545	ASN	CB-CA-C	7.11	124.89	110.38
1	A	482	ILE	CA-C-O	6.97	128.56	121.17
1	B	497	THR	O-C-N	6.96	132.08	123.10
1	B	498	ASP	CA-C-N	6.96	131.67	122.42
1	B	498	ASP	C-N-CA	6.96	131.67	122.42
1	B	489	SER	CA-C-O	-6.86	111.63	120.00
1	B	500	GLN	CA-C-N	6.80	129.29	120.44
1	B	500	GLN	C-N-CA	6.80	129.29	120.44
1	A	489	SER	CA-C-N	-6.80	108.08	121.41
1	A	489	SER	C-N-CA	-6.80	108.08	121.41
1	A	505	ILE	CB-CA-C	-6.79	103.11	111.87
1	B	511	ASP	N-CA-C	-6.75	97.47	110.56
1	B	475	GLN	OE1-CD-NE2	-6.73	115.87	122.60
1	A	552	VAL	CB-CA-C	6.71	121.24	112.24
1	A	552	VAL	N-CA-CB	-6.69	99.39	110.56
1	B	460	ASN	CB-CG-ND2	6.60	126.31	116.40
1	B	470	THR	CA-CB-OG1	-6.59	99.72	109.60
1	A	481	ALA	O-C-N	-6.58	115.24	122.09
1	A	493	VAL	N-CA-C	6.52	118.09	108.45
1	A	547	GLN	N-CA-C	-6.49	104.13	111.07
1	A	497	THR	CA-C-N	-6.45	112.44	122.37
1	A	497	THR	C-N-CA	-6.45	112.44	122.37
1	A	489	SER	N-CA-C	6.37	121.46	113.43
1	A	526	ILE	O-C-N	6.37	128.16	121.91
1	A	493	VAL	CB-CA-C	-6.34	99.73	110.71
1	A	529	GLU	CA-C-O	6.33	127.32	120.55
1	A	524	GLN	OE1-CD-NE2	6.32	128.91	122.60
1	A	491	LEU	CA-C-O	-6.31	112.16	119.61
1	B	455	ALA	CA-C-N	-6.29	109.07	121.41
1	B	455	ALA	C-N-CA	-6.29	109.07	121.41
1	B	528	LYS	CA-CB-CG	6.29	126.67	114.10
1	A	442	VAL	CB-CA-C	6.26	120.14	111.49
1	B	536	VAL	O-C-N	6.26	128.24	121.10
1	B	513	SER	CA-C-N	-6.23	112.26	122.54
1	B	513	SER	C-N-CA	-6.23	112.26	122.54
1	A	442	VAL	N-CA-CB	-6.23	99.96	111.91
1	B	491	LEU	N-CA-C	6.22	119.97	112.38
1	A	439	THR	O-C-N	6.21	130.28	123.27
1	A	472	THR	N-CA-CB	-6.17	101.62	111.62
1	A	474	ASN	CA-C-N	6.17	129.05	120.29
1	A	474	ASN	C-N-CA	6.17	129.05	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	489	SER	CA-C-N	-6.15	109.35	121.41
1	B	489	SER	C-N-CA	-6.15	109.35	121.41
1	B	469	LEU	N-CA-CB	-6.15	101.01	110.85
1	B	442	VAL	CG1-CB-CG2	6.11	124.25	110.80
1	B	464	GLN	N-CA-CB	-6.11	101.46	111.66
1	B	465	LYS	CA-C-N	6.06	131.53	122.75
1	B	465	LYS	C-N-CA	6.06	131.53	122.75
1	A	458	VAL	CA-C-O	-6.05	113.84	120.43
1	B	516	GLU	O-C-N	6.03	128.60	122.09
1	B	517	LEU	CA-C-O	-5.97	114.18	120.63
1	B	496	VAL	N-CA-C	5.96	116.20	106.72
1	B	490	GLY	CA-C-N	5.95	130.12	120.60
1	B	490	GLY	C-N-CA	5.95	130.12	120.60
1	A	433	PRO	CA-C-N	5.92	130.09	121.80
1	A	433	PRO	C-N-CA	5.92	130.09	121.80
1	A	536	VAL	CA-C-O	-5.92	114.73	121.59
1	B	467	VAL	O-C-N	5.91	127.84	121.10
1	A	494	ASN	CA-C-N	-5.90	115.49	123.10
1	A	494	ASN	C-N-CA	-5.90	115.49	123.10
1	B	492	GLU	CB-CG-CD	5.88	122.59	112.60
1	A	523	GLU	N-CA-C	-5.88	104.88	111.28
1	B	464	GLN	CB-CG-CD	-5.86	102.63	112.60
1	B	514	GLU	CB-CA-C	5.84	119.85	110.09
1	A	454	LYS	CA-C-O	5.78	127.64	121.11
1	B	478	GLU	CA-C-N	-5.78	112.09	120.29
1	B	478	GLU	C-N-CA	-5.78	112.09	120.29
1	A	451	LYS	CA-C-O	5.75	128.12	121.28
1	A	552	VAL	CA-C-N	5.75	128.56	120.28
1	A	552	VAL	C-N-CA	5.75	128.56	120.28
1	B	473	THR	CA-C-O	-5.75	114.72	121.44
1	A	477	THR	CA-C-N	5.73	127.96	120.28
1	A	477	THR	C-N-CA	5.73	127.96	120.28
1	A	434	ILE	CA-C-N	5.73	128.77	120.98
1	A	434	ILE	C-N-CA	5.73	128.77	120.98
1	B	438	GLU	CB-CG-CD	5.72	122.33	112.60
1	A	468	PRO	N-CA-CB	-5.72	97.25	103.25
1	A	489	SER	O-C-N	-5.72	114.44	122.10
1	B	531	VAL	N-CA-CB	-5.66	103.26	111.52
1	B	493	VAL	CA-C-O	-5.66	116.03	121.63
1	B	524	GLN	OE1-CD-NE2	5.65	128.25	122.60
1	B	460	ASN	CA-CB-CG	-5.64	106.96	112.60
1	A	547	GLN	O-C-N	5.64	127.88	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	497	THR	O-C-N	5.63	130.80	122.97
1	B	459	THR	CA-CB-OG1	-5.63	101.15	109.60
1	A	490	GLY	CA-C-N	5.62	129.69	120.63
1	A	490	GLY	C-N-CA	5.62	129.69	120.63
1	A	517	LEU	O-C-N	5.62	128.09	122.08
1	A	466	VAL	O-C-N	5.52	129.37	123.03
1	A	503	LEU	CA-C-N	5.50	127.21	120.22
1	A	503	LEU	C-N-CA	5.50	127.21	120.22
1	A	464	GLN	O-C-N	5.49	129.51	123.25
1	B	494	ASN	CA-C-N	-5.49	114.80	122.71
1	B	494	ASN	C-N-CA	-5.49	114.80	122.71
1	B	490	GLY	N-CA-C	-5.49	100.17	113.18
1	B	440	PHE	CA-C-O	-5.49	114.49	120.36
1	B	515	SER	N-CA-CB	5.49	119.21	110.16
1	A	483	TYR	O-C-N	5.48	127.79	122.09
1	B	447	ASN	O-C-N	5.48	129.47	123.22
1	A	536	VAL	N-CA-CB	-5.46	105.79	111.64
1	B	502	ALA	O-C-N	-5.46	115.92	122.15
1	A	466	VAL	CA-C-O	-5.46	114.80	120.64
1	A	475	GLN	OE1-CD-NE2	-5.45	117.15	122.60
1	B	458	VAL	CB-CA-C	5.42	120.18	111.29
1	A	516	GLU	O-C-N	5.41	127.71	122.09
1	B	530	LYS	N-CA-CB	5.40	119.68	110.71
1	B	552	VAL	CB-CA-C	5.38	119.24	111.65
1	A	549	ASP	CA-C-O	5.38	126.65	121.00
1	B	493	VAL	O-C-N	5.30	129.01	123.02
1	A	496	VAL	O-C-N	5.30	128.17	123.03
1	A	554	ALA	CA-C-N	5.29	129.93	122.63
1	A	554	ALA	C-N-CA	5.29	129.93	122.63
1	A	464	GLN	CB-CA-C	-5.28	99.09	110.45
1	B	496	VAL	CA-C-O	-5.26	113.85	120.69
1	B	442	VAL	CA-C-O	-5.24	115.14	121.54
1	A	433	PRO	N-CA-C	-5.23	102.98	111.03
1	A	526	ILE	CA-C-O	-5.21	115.64	121.17
1	A	497	THR	N-CA-CB	5.18	118.42	110.70
1	A	523	GLU	CB-CG-CD	5.18	121.40	112.60
1	A	521	ILE	CA-C-O	5.17	126.42	121.05
1	B	497	THR	CA-C-O	-5.16	115.32	121.56
1	A	443	ASP	CA-C-O	5.16	126.78	121.06
1	B	462	GLY	CA-C-N	5.12	128.14	120.87
1	B	462	GLY	C-N-CA	5.12	128.14	120.87
1	B	457	TYR	CA-C-O	5.08	126.75	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	459	THR	CA-CB-CG2	5.08	119.13	110.50
1	B	465	LYS	N-CA-C	5.07	116.12	108.46
1	B	454	LYS	O-C-N	5.04	129.43	123.33
1	A	463	ARG	NE-CZ-NH2	-5.04	114.66	119.20
1	B	478	GLU	CB-CG-CD	5.04	121.16	112.60
1	A	487	GLN	CB-CG-CD	-5.03	104.05	112.60

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	57	0
1	B	882	0	838	39	0
All	All	1803	0	1739	96	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 27.

All (96) 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:B:460:ASN:OD1	1:B:460:ASN:C	2.38	0.61
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.02	0.59
1:A:516:GLU:O	1:A:520:GLN:HG3	2.03	0.58
1:A:457:TYR:C	1:A:457:TYR:CD1	2.80	0.58
1:A:427:TYR:OH	1:A:509:GLN:HA	2.03	0.58
1:A:461:LYS:HZ1	1:A:461:LYS:HA	1.68	0.57
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: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:O	1:B:470:THR:HG23	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:522:ILE:O	1:A:526:ILE:HG13	2.10	0.52
1:A:463:ARG:HB2	1:A:463:ARG:NH1	2.20	0.52
1:A:461:LYS:HA	1:A:461:LYS:NZ	2.25	0.51
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:A:549:ASP:O	1:A:550:LYS:C	2.54	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: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:470:THR:O	1:B:471:ASN:C	2.54	0.48
1:B:517:LEU:O	1:B:520:GLN:HB2	2.14	0.47
1:B:518:VAL:O	1:B:522:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:TRP:CH2	1:A:537:PRO:HB3	2.49	0.47
1:A:517:LEU:HD23	1:A:517:LEU:HA	1.53	0.47
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: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:473:THR:O	1:B:477:THR:HG23	2.16	0.45
1:B:489:SER:HB2	1:B:493:VAL:HG13	1.97	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: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:B:502:ALA:O	1:B:503:LEU:C	2.60	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:457:TYR:C	1:B:458:VAL:HG23	2.42	0.43
1:B:447:ASN:O	1:B:451:LYS:HA	2.18	0.43
1:B:535:TRP:O	1:B:536:VAL:CG2	2.64	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:A:480:GLN:O	1:A:481:ALA:C	2.60	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:B:474:ASN:O	1:B:475:GLN:C	2.63	0.41
1:A:443:ASP:O	1:A:481:ALA:HB2	2.20	0.41
1:A:497:THR:O	1:A:535:TRP:HA	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:A:492:GLU:HG2	1:A:530:LYS:HB2	2.01	0.41
1:B:451:LYS:O	1:B:471:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:LEU:C	1:A:430:GLU:O	2.60	0.41
1:A:447:ASN:O	1:A:451:LYS:N	2.45	0.41
1:A:523:GLU:HG2	1:A:524:GLN:N	2.36	0.41
1:A:523:GLU:CG	1:A:524:GLN:N	2.84	0.40
1:A:496:VAL:O	1:A:496:VAL:CG2	2.70	0.40
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%)	74 (80%)	19 (20%)	1	1
1	B	86/114 (75%)	70 (81%)	16 (19%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	179/228 (78%)	144 (80%)	35 (20%)	1 2

All (35) 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	467	VAL
1	A	468	PRO
1	A	470	THR
1	A	479	LEU
1	A	484	LEU
1	A	493	VAL
1	A	496	VAL
1	A	497	THR
1	A	505	ILE
1	A	517	LEU
1	A	522	ILE
1	A	530	LYS
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	458	VAL
1	B	470	THR
1	B	479	LEU
1	B	484	LEU
1	B	493	VAL
1	B	497	THR
1	B	509	GLN
1	B	513	SER
1	B	531	VAL
1	B	533	LEU
1	B	536	VAL
1	B	552	VAL
1	B	553	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	475	GLN
1	A	520	GLN
1	A	547	GLN
1	B	480	GLN
1	B	507	GLN
1	B	520	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 oligosaccharides 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 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.