



# Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1DB2 / pdb\_00001db2  
Title : CRYSTAL STRUCTURE OF NATIVE PLASMINOGEN ACTIVATOR INHIBITOR-1  
Authors : Nar, H.; Bauer, M.; Stassen, J.M.; Lang, D.; Gils, A.; Declerck, P.  
Deposited on : 1999-11-02  
Resolution : 2.70 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

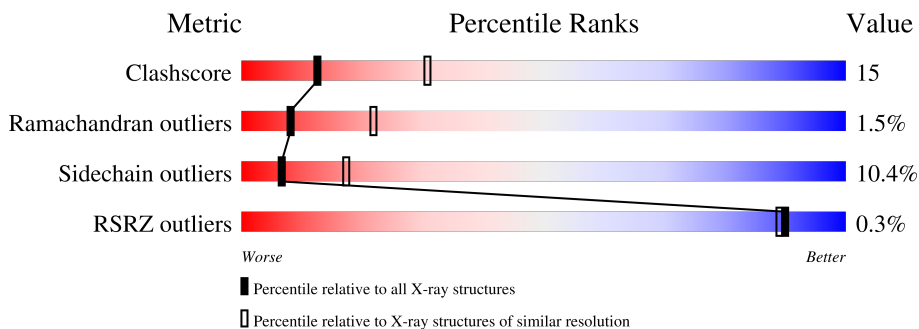
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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.

Mol	Chain	Length	Quality of chain
1	A	377	 56% 33% 8% .
1	B	377	 55% 35% 5% . .

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5887 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 PLASMINOGEN ACTIVATOR INHIBITOR-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	377	2993	1921	510	547	15	0	0	0
1	B	362	2894	1861	492	527	14	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	150	HIS	ASN	engineered mutation	UNP P05121
A	154	THR	LYS	engineered mutation	UNP P05121
A	301	PRO	GLN	engineered mutation	UNP P05121
A	319	LEU	GLN	engineered mutation	UNP P05121
A	354	ILE	MET	engineered mutation	UNP P05121
B	150	HIS	ASN	engineered mutation	UNP P05121
B	154	THR	LYS	engineered mutation	UNP P05121
B	301	PRO	GLN	engineered mutation	UNP P05121
B	319	LEU	GLN	engineered mutation	UNP P05121
B	354	ILE	MET	engineered mutation	UNP P05121



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.60Å 92.60Å 251.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.1 (20.00-2.70) 95.8 (20.00-2.70)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.14 (at 2.55Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.255 , 0.299 0.188 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.2	Xtrriage
Anisotropy	0.279	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 4.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	0.289 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5887	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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	1.05	6/3068 (0.2%)	1.94	93/4164 (2.2%)
1	B	0.90	3/2968 (0.1%)	1.90	71/4025 (1.8%)
All	All	0.98	9/6036 (0.1%)	1.92	164/8189 (2.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	HIS	C-N	18.37	1.55	1.33
1	A	3	HIS	CB-CG	7.91	1.61	1.50
1	B	7	TYR	C-N	-6.96	1.25	1.33
1	B	379	PRO	C-O	6.56	1.36	1.23
1	A	379	PRO	C-OXT	6.35	1.36	1.23
1	A	3	HIS	CA-CB	6.22	1.65	1.53
1	A	379	PRO	C-O	5.99	1.35	1.23
1	B	379	PRO	C-OXT	5.87	1.35	1.23
1	A	3	HIS	CG-CD2	5.04	1.41	1.35

All (164) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	3	HIS	CA-C-N	13.81	134.61	120.38
1	A	3	HIS	C-N-CA	13.81	134.61	120.38
1	B	6	SER	CA-C-N	11.52	135.71	120.28
1	B	6	SER	C-N-CA	11.52	135.71	120.28
1	A	300	ARG	CA-C-O	11.40	129.00	119.66
1	A	129	VAL	N-CA-C	10.60	121.44	110.62
1	A	194	GLY	N-CA-C	-10.33	102.19	114.48
1	B	10	HIS	CA-CB-CG	-10.18	103.62	113.80
1	A	303	GLN	CA-CB-CG	9.91	133.92	114.10
1	B	137	ASN	CA-CB-CG	-9.71	102.89	112.60
1	A	341	VAL	CB-CA-C	9.53	119.59	110.63
1	B	18	ARG	NE-CZ-NH1	-9.36	112.14	121.50
1	B	129	VAL	N-CA-C	9.23	120.03	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	328	VAL	O-C-N	9.03	131.47	122.71
1	B	6	SER	CA-C-O	8.76	130.18	119.31
1	A	10	HIS	CA-CB-CG	-8.53	105.28	113.80
1	A	4	PRO	CA-C-N	8.36	130.29	119.84
1	A	4	PRO	C-N-CA	8.36	130.29	119.84
1	A	5	PRO	CA-C-N	7.88	136.63	122.38
1	A	5	PRO	C-N-CA	7.88	136.63	122.38
1	A	218	GLY	N-CA-C	7.87	126.23	115.30
1	B	179	PHE	CA-CB-CG	7.86	121.66	113.80
1	A	5	PRO	O-C-N	-7.86	112.03	122.64
1	B	311	ASP	CA-CB-CG	-7.69	104.91	112.60
1	A	109	PHE	CA-CB-CG	-7.64	106.16	113.80
1	A	285	ASP	CA-CB-CG	-7.61	104.99	112.60
1	A	303	GLN	N-CA-CB	-7.51	100.60	110.59
1	B	5	PRO	CA-C-O	-7.46	107.01	120.60
1	B	133	ARG	NE-CZ-NH2	-7.46	112.48	119.20
1	A	5	PRO	CB-CA-C	7.40	123.77	111.56
1	B	218	GLY	N-CA-C	7.38	126.45	115.08
1	A	311	ASP	CA-CB-CG	-7.33	105.27	112.60
1	B	363	ARG	CD-NE-CZ	-7.25	114.24	124.40
1	A	3	HIS	CB-CA-C	7.25	123.87	110.10
1	B	64	PHE	CA-CB-CG	7.17	120.97	113.80
1	B	94	THR	N-CA-CB	7.12	124.08	111.69
1	B	201	MET	CA-C-O	-7.02	113.22	121.16
1	B	303	GLN	CA-CB-CG	7.01	128.12	114.10
1	B	5	PRO	N-CA-C	7.01	126.91	112.47
1	A	101	ARG	N-CA-C	7.00	119.80	111.33
1	A	155	GLY	CA-C-O	-6.98	113.96	120.80
1	A	192	SER	CA-C-N	6.91	129.53	120.28
1	A	192	SER	C-N-CA	6.91	129.53	120.28
1	A	278	PHE	CA-CB-CG	6.90	120.70	113.80
1	A	94	THR	N-CA-CB	6.86	123.48	111.55
1	B	193	ASP	CB-CA-C	-6.78	100.24	110.88
1	B	129	VAL	CA-C-O	-6.65	114.03	120.95
1	B	18	ARG	NE-CZ-NH2	6.64	125.17	119.20
1	B	322	GLN	CB-CG-CD	6.63	123.87	112.60
1	B	367	THR	CA-C-O	6.60	126.31	119.05
1	A	157	VAL	N-CA-CB	6.58	118.31	110.95
1	A	3	HIS	CB-CG-CD2	-6.46	122.81	131.20
1	A	352	ILE	N-CA-CB	6.46	120.03	112.35
1	B	154	THR	CA-C-N	6.43	128.23	120.13
1	B	154	THR	C-N-CA	6.43	128.23	120.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	THR	CA-C-O	6.42	126.87	120.32
1	B	192	SER	CA-C-N	6.42	128.79	120.44
1	B	192	SER	C-N-CA	6.42	128.79	120.44
1	B	328	VAL	CB-CA-C	-6.42	103.97	111.09
1	A	45	MET	CA-C-O	6.36	127.50	120.82
1	A	8	VAL	CA-C-O	-6.31	114.48	121.17
1	A	130	GLU	CB-CG-CD	6.30	123.31	112.60
1	A	3	HIS	CB-CG-ND1	6.29	132.14	122.70
1	A	7	TYR	N-CA-C	-6.27	104.53	111.36
1	A	187	ARG	NE-CZ-NH2	-6.26	113.56	119.20
1	A	69	LYS	CA-CB-CG	6.25	126.60	114.10
1	B	277	LYS	CA-C-O	-6.25	114.75	121.56
1	B	303	GLN	N-CA-C	-6.25	105.56	113.43
1	B	105	LEU	CA-C-O	-6.19	114.35	121.47
1	A	313	GLU	CB-CG-CD	6.16	123.08	112.60
1	B	7	TYR	N-CA-CB	-6.16	101.07	110.12
1	B	179	PHE	N-CA-C	-6.16	102.30	109.93
1	A	330	GLU	N-CA-C	6.14	118.05	111.36
1	A	332	GLY	N-CA-C	-6.13	106.50	115.63
1	A	378	GLU	CA-C-O	6.11	128.53	120.16
1	A	158	ASP	CA-CB-CG	6.10	118.70	112.60
1	A	193	ASP	CB-CA-C	-6.10	100.66	110.79
1	A	61	ALA	CA-C-O	-6.10	113.47	120.24
1	A	5	PRO	CA-N-CD	-6.07	103.50	112.00
1	A	174	GLN	CA-C-O	-6.07	113.86	120.36
1	B	332	GLY	N-CA-C	-6.06	106.79	115.64
1	A	21	GLN	CB-CG-CD	-6.06	102.31	112.60
1	B	274	VAL	N-CA-CB	6.04	119.50	111.64
1	A	280	LEU	CA-C-N	6.01	131.29	122.39
1	A	280	LEU	C-N-CA	6.01	131.29	122.39
1	B	206	ASN	OD1-CG-ND2	-5.99	116.61	122.60
1	B	29	ASP	CB-CA-C	5.99	115.76	109.83
1	A	371	LEU	CA-C-O	-5.96	114.17	120.55
1	B	109	PHE	CA-CB-CG	-5.94	107.86	113.80
1	A	287	ARG	CD-NE-CZ	5.85	132.59	124.40
1	A	278	PHE	O-C-N	5.83	129.23	123.46
1	A	277	LYS	N-CA-C	-5.82	102.84	110.53
1	A	129	VAL	O-C-N	-5.81	116.24	121.87
1	A	207	LYS	N-CA-C	-5.80	99.73	108.96
1	B	328	VAL	N-CA-CB	5.78	119.23	112.35
1	B	29	ASP	CA-CB-CG	-5.77	106.83	112.60
1	B	151	LEU	CA-C-O	-5.76	114.08	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	THR	CA-C-N	5.73	130.50	122.08
1	A	144	THR	C-N-CA	5.73	130.50	122.08
1	A	95	ASP	CA-C-O	-5.69	114.11	120.66
1	B	21	GLN	OE1-CD-NE2	5.69	128.29	122.60
1	A	192	SER	CA-C-O	5.64	125.35	119.14
1	A	232	THR	N-CA-C	-5.63	104.53	111.40
1	B	70	GLY	N-CA-C	5.63	122.83	115.40
1	A	221	TYR	CA-CB-CG	5.61	124.00	113.90
1	A	287	ARG	N-CA-C	5.60	117.86	111.02
1	A	3	HIS	CA-CB-CG	-5.60	108.20	113.80
1	A	91	ILE	N-CA-C	5.60	116.13	107.78
1	B	297	ASP	N-CA-C	5.58	117.36	111.28
1	B	176	LYS	CA-C-N	5.57	128.98	122.52
1	B	176	LYS	C-N-CA	5.57	128.98	122.52
1	A	303	GLN	OE1-CD-NE2	5.55	128.16	122.60
1	B	378	GLU	CA-C-O	5.50	127.69	120.16
1	A	70	GLY	N-CA-C	5.49	121.62	115.08
1	B	193	ASP	CA-C-O	5.48	126.57	120.82
1	B	249	ALA	N-CA-C	-5.46	105.44	111.71
1	B	224	LEU	CA-C-O	-5.43	114.83	120.70
1	B	322	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	A	4	PRO	CA-N-CD	-5.40	104.44	112.00
1	A	138	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	92	SER	CA-C-O	-5.39	115.02	121.11
1	A	29	ASP	CA-CB-CG	-5.39	107.21	112.60
1	B	330	GLU	N-CA-C	5.38	117.14	111.28
1	A	179	PHE	CA-CB-CG	5.36	119.16	113.80
1	B	303	GLN	OE1-CD-NE2	5.34	127.94	122.60
1	A	310	SER	N-CA-C	5.34	116.64	108.42
1	B	6	SER	N-CA-CB	5.34	119.10	110.40
1	B	313	GLU	CB-CG-CD	5.32	121.65	112.60
1	B	277	LYS	N-CA-C	-5.32	103.00	110.50
1	B	208	PHE	CA-CB-CG	5.31	119.11	113.80
1	B	353	ILE	CA-C-N	-5.31	116.12	122.22
1	B	353	ILE	C-N-CA	-5.31	116.12	122.22
1	B	307	THR	CA-C-O	-5.30	112.16	119.05
1	A	139	TRP	N-CA-C	-5.29	105.20	110.97
1	A	303	GLN	CA-C-O	5.29	125.22	119.24
1	A	342	ILE	N-CA-C	5.29	115.96	107.98
1	A	290	LEU	CB-CA-C	5.26	119.22	110.90
1	B	101	ARG	N-CA-C	5.26	117.42	111.11
1	A	279	SER	N-CA-CB	-5.24	102.25	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	HIS	CA-C-O	5.22	127.08	121.55
1	A	363	ARG	N-CA-C	5.21	118.06	109.72
1	A	132	ALA	O-C-N	5.21	127.65	122.08
1	A	112	HIS	CA-C-N	5.21	127.52	120.44
1	A	112	HIS	C-N-CA	5.21	127.52	120.44
1	A	301	PRO	N-CD-CG	-5.20	95.40	103.20
1	A	12	ALA	O-C-N	5.19	127.63	122.08
1	B	18	ARG	CD-NE-CZ	-5.17	117.17	124.40
1	A	48	LEU	N-CA-C	5.16	117.64	111.71
1	A	33	VAL	O-C-N	-5.14	117.89	123.14
1	A	5	PRO	N-CA-C	5.12	123.02	112.47
1	B	352	ILE	N-CA-CB	5.10	118.63	112.10
1	B	139	TRP	N-CA-C	-5.09	105.42	110.97
1	B	242	GLU	N-CA-C	5.08	117.04	108.96
1	A	125	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	313	GLU	CA-C-O	-5.07	113.22	120.16
1	B	303	GLN	CA-C-O	5.06	125.66	119.64
1	A	286	LEU	N-CA-C	5.06	118.71	112.54
1	A	196	THR	N-CA-CB	-5.04	102.93	111.69
1	B	5	PRO	O-C-N	-5.03	115.85	122.64
1	B	271	ARG	CA-CB-CG	5.03	124.16	114.10
1	A	312	GLN	CA-C-O	5.03	126.23	120.80
1	B	115	ARG	N-CA-C	-5.02	105.69	111.07
1	A	121	VAL	CA-C-O	-5.02	115.13	120.85
1	B	310	SER	N-CA-C	5.01	116.14	108.42

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	2993	0	2987	89	0
1	B	2894	0	2880	96	0
All	All	5887	0	5867	180	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 (180) 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:3:HIS:N	1:A:4:PRO:HD2	1.60	1.14
1:A:3:HIS:O	1:A:7:TYR:HB2	1.55	1.05
1:B:206:ASN:HD22	1:B:207:LYS:N	1.56	1.03
1:A:206:ASN:HD22	1:A:207:LYS:H	1.02	1.00
1:A:3:HIS:HB2	1:A:7:TYR:CD2	2.05	0.91
1:A:3:HIS:N	1:A:4:PRO:CD	2.35	0.90
1:B:206:ASN:HD22	1:B:207:LYS:H	0.90	0.87
1:A:206:ASN:HD22	1:A:207:LYS:N	1.76	0.84
1:B:206:ASN:ND2	1:B:207:LYS:H	1.75	0.84
1:B:100:GLN:HE22	1:B:126:PHE:H	1.30	0.77
1:A:206:ASN:ND2	1:A:207:LYS:H	1.82	0.77
1:A:100:GLN:HE22	1:A:126:PHE:H	1.33	0.76
1:B:248:SER:HA	1:B:251:THR:HB	1.68	0.75
1:A:167:ASN:HD22	1:A:322:GLN:HE21	1.33	0.73
1:B:215:THR:HB	1:B:216:PRO:HD2	1.73	0.71
1:B:110:MET:HB2	1:B:111:PRO:HD3	1.73	0.70
1:A:110:MET:HB2	1:A:111:PRO:HD3	1.73	0.70
1:B:72:ALA:HB3	1:B:73:PRO:HD3	1.75	0.69
1:B:45:MET:HE3	1:B:113:PHE:HZ	1.57	0.68
1:A:248:SER:HA	1:A:251:THR:HB	1.74	0.68
1:B:167:ASN:HD22	1:B:322:GLN:HE21	1.43	0.66
1:A:3:HIS:HB2	1:A:7:TYR:CG	2.31	0.66
1:B:4:PRO:HB2	1:B:5:PRO:CD	2.27	0.65
1:A:101:ARG:HG2	1:A:123:GLN:HB3	1.79	0.64
1:A:347:MET:HE2	1:B:325:LYS:HE3	1.80	0.63
1:A:210:TYR:HD2	1:A:224:LEU:HD23	1.64	0.62
1:B:287:ARG:O	1:B:291:GLU:HG3	1.98	0.62
1:B:206:ASN:ND2	1:B:207:LYS:N	2.39	0.62
1:B:283:GLU:HB2	1:B:323:LYS:HD2	1.80	0.62
1:A:3:HIS:O	1:A:7:TYR:CB	2.43	0.61
1:A:215:THR:HB	1:A:216:PRO:HD2	1.83	0.60
1:B:4:PRO:HG2	1:B:7:TYR:HD2	1.66	0.60
1:A:28:LYS:O	1:A:29:ASP:HB2	2.02	0.60
1:A:72:ALA:HB3	1:A:73:PRO:HD3	1.83	0.60
1:B:100:GLN:NE2	1:B:126:PHE:H	1.97	0.60
1:B:180:PRO:HG2	1:B:183:SER:OG	2.02	0.60
1:B:272:LEU:HD12	1:B:351:GLU:HG2	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:LYS:HB2	1:B:289:PRO:HD3	1.84	0.59
1:B:100:GLN:HE21	1:B:126:PHE:HB2	1.67	0.59
1:B:53:GLU:O	1:B:57:GLN:HG3	2.02	0.59
1:B:210:TYR:HD2	1:B:224:LEU:HD23	1.67	0.59
1:A:288:LYS:HB2	1:A:289:PRO:HD3	1.85	0.59
1:A:272:LEU:HD12	1:A:351:GLU:HG2	1.85	0.59
1:A:122:LYS:HE3	1:A:139:TRP:CH2	2.38	0.58
1:B:45:MET:HE3	1:B:113:PHE:CZ	2.38	0.58
1:B:300:ARG:CB	1:B:303:GLN:HG3	2.34	0.57
1:B:47:GLN:HE22	1:B:65:LYS:HA	1.70	0.57
1:B:101:ARG:HG2	1:B:123:GLN:HB3	1.86	0.57
1:A:287:ARG:O	1:A:291:GLU:HG3	2.05	0.57
1:B:122:LYS:HE3	1:B:139:TRP:CH2	2.39	0.57
1:B:227:PRO:HA	1:B:234:SER:HB3	1.87	0.56
1:A:100:GLN:NE2	1:A:126:PHE:H	2.00	0.56
1:B:100:GLN:NE2	1:B:126:PHE:HB2	2.20	0.56
1:A:341:VAL:CG2	1:B:289:PRO:HD3	2.36	0.55
1:A:45:MET:HE3	1:A:113:PHE:HZ	1.72	0.54
1:B:131:ARG:O	1:B:135:ILE:HG12	2.06	0.54
1:A:29:ASP:HA	1:A:377:MET:HE2	1.90	0.54
1:A:167:ASN:HD22	1:A:322:GLN:NE2	2.03	0.54
1:B:209:ASN:ND2	1:B:268:ARG:HG2	2.23	0.54
1:B:28:LYS:O	1:B:29:ASP:HB2	2.07	0.53
1:B:186:ARG:O	1:B:187:ARG:HB2	2.09	0.53
1:A:167:ASN:ND2	1:A:322:GLN:HE21	2.02	0.53
1:A:199:VAL:HG11	1:A:379:PRO:O	2.08	0.52
1:B:127:SER:HA	1:B:159:GLN:HG2	1.91	0.52
1:A:100:GLN:HE21	1:A:126:PHE:HB2	1.75	0.52
1:B:193:ASP:HB3	1:B:195:SER:H	1.73	0.52
1:A:247:LEU:HD21	1:A:359:LEU:HD13	1.91	0.51
1:B:205:THR:CG2	1:B:272:LEU:HD23	2.40	0.51
1:A:13:SER:O	1:A:17:VAL:HG23	2.10	0.51
1:B:38:GLY:HA3	1:B:167:ASN:HD21	1.75	0.51
1:B:300:ARG:HB3	1:B:303:GLN:HG3	1.92	0.51
1:A:100:GLN:NE2	1:A:126:PHE:HB2	2.26	0.51
1:A:131:ARG:O	1:A:135:ILE:HG12	2.10	0.51
1:A:171:PHE:HB2	1:A:372:PHE:CZ	2.46	0.50
1:A:341:VAL:HG21	1:B:289:PRO:HD3	1.93	0.50
1:B:48:LEU:HD12	1:B:113:PHE:CD1	2.46	0.50
1:B:122:LYS:N	1:B:122:LYS:HD2	2.27	0.50
1:A:313:GLU:HA	1:A:313:GLU:OE2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ASN:CG	1:A:91:ILE:HG22	2.37	0.50
1:A:110:MET:HA	1:A:110:MET:HE2	1.94	0.49
1:B:100:GLN:HE22	1:B:126:PHE:N	2.04	0.49
1:B:82:LEU:HA	1:B:86:TRP:HZ2	1.78	0.49
1:A:347:MET:HE2	1:B:325:LYS:CE	2.42	0.49
1:A:254:LEU:HD13	1:A:373:MET:HE2	1.93	0.49
1:A:206:ASN:ND2	1:A:207:LYS:N	2.49	0.48
1:A:101:ARG:HB3	1:A:101:ARG:HH11	1.79	0.48
1:A:305:ASP:OD1	1:A:307:THR:HG23	2.14	0.48
1:B:122:LYS:HE3	1:B:139:TRP:CZ3	2.48	0.48
1:A:168:ALA:HA	1:A:323:LYS:O	2.14	0.48
1:A:3:HIS:N	1:A:3:HIS:CD2	2.81	0.47
1:B:64:PHE:HB2	1:B:71:MET:HE2	1.95	0.47
1:A:326:ILE:O	1:A:326:ILE:HG23	2.15	0.47
1:B:205:THR:HG22	1:B:272:LEU:HA	1.96	0.47
1:B:356:ARG:O	1:B:357:PRO:C	2.56	0.47
1:A:245:VAL:O	1:A:356:ARG:NH2	2.48	0.47
1:B:4:PRO:CB	1:B:5:PRO:HD3	2.45	0.46
1:B:181:ASP:O	1:B:183:SER:N	2.48	0.46
1:B:205:THR:HG23	1:B:272:LEU:HD23	1.97	0.46
1:A:38:GLY:HA3	1:A:167:ASN:HD21	1.81	0.46
1:B:205:THR:HG22	1:B:272:LEU:HB2	1.97	0.46
1:A:207:LYS:HG3	1:A:346:ARG:CZ	2.46	0.46
1:B:168:ALA:HA	1:B:323:LYS:O	2.16	0.46
1:A:230:GLY:O	1:A:231:ASP:HB2	2.15	0.46
1:A:300:ARG:HA	1:A:301:PRO:HD3	1.55	0.46
1:A:356:ARG:HB2	1:A:357:PRO:HD2	1.97	0.46
1:A:165:LEU:C	1:A:165:LEU:HD12	2.41	0.46
1:A:301:PRO:HG3	1:A:316:HIS:CE1	2.51	0.46
1:B:117:PHE:O	1:B:118:ARG:HB2	2.16	0.46
1:B:361:VAL:HG22	1:B:373:MET:HE3	1.97	0.46
1:B:110:MET:HA	1:B:110:MET:HE2	1.97	0.45
1:B:300:ARG:HB2	1:B:303:GLN:HG3	1.98	0.45
1:B:262:TRP:O	1:B:266:MET:HG3	2.16	0.45
1:B:72:ALA:N	1:B:73:PRO:CD	2.79	0.45
1:B:313:GLU:HB3	1:B:314:PRO:HD3	1.97	0.45
1:B:4:PRO:CB	1:B:5:PRO:CD	2.90	0.45
1:B:275:LEU:HA	1:B:276:PRO:HD3	1.88	0.45
1:A:8:VAL:HG12	1:A:71:MET:HE1	1.98	0.45
1:B:151:LEU:HD12	1:B:323:LYS:HD3	1.99	0.45
1:A:262:TRP:O	1:A:266:MET:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:ASN:CG	1:B:91:ILE:HG22	2.42	0.44
1:B:109:PHE:CD2	1:B:109:PHE:C	2.95	0.44
1:A:4:PRO:O	1:A:6:SER:N	2.31	0.44
1:A:254:LEU:HD13	1:A:373:MET:CE	2.47	0.44
1:B:245:VAL:O	1:B:356:ARG:NH2	2.50	0.44
1:B:205:THR:HG22	1:B:272:LEU:CB	2.47	0.44
1:A:162:ARG:HH12	1:A:314:PRO:HD2	1.83	0.44
1:A:193:ASP:HB3	1:A:195:SER:H	1.83	0.44
1:B:139:TRP:CD1	1:B:139:TRP:C	2.95	0.44
1:B:167:ASN:HD22	1:B:322:GLN:NE2	2.11	0.44
1:A:91:ILE:CD1	1:A:371:LEU:HD13	2.48	0.44
1:A:122:LYS:HD2	1:A:122:LYS:N	2.32	0.44
1:A:361:VAL:HG22	1:A:373:MET:HE3	2.00	0.44
1:A:101:ARG:HB3	1:A:101:ARG:NH1	2.32	0.43
1:A:315:LEU:HD23	1:A:315:LEU:HA	1.90	0.43
1:B:90:GLU:O	1:B:171:PHE:HA	2.18	0.43
1:A:90:GLU:O	1:A:171:PHE:HA	2.18	0.43
1:A:313:GLU:HB3	1:A:314:PRO:HD3	2.00	0.43
1:B:167:ASN:O	1:B:322:GLN:HA	2.18	0.43
1:B:356:ARG:HB2	1:B:357:PRO:HD2	2.00	0.43
1:A:349:PRO:HG2	1:A:350:GLU:H	1.82	0.43
1:B:211:THR:HG23	1:B:223:ILE:HD13	2.00	0.43
1:B:94:THR:HG21	1:B:139:TRP:HE1	1.82	0.43
1:B:185:HIS:H	1:B:185:HIS:HD1	1.67	0.43
1:B:247:LEU:HD12	1:B:247:LEU:HA	1.84	0.43
1:A:46:LEU:HD12	1:A:46:LEU:HA	1.87	0.43
1:A:167:ASN:ND2	1:A:322:GLN:NE2	2.65	0.43
1:B:259:ILE:HD11	1:B:373:MET:HE1	1.99	0.43
1:A:5:PRO:O	1:A:8:VAL:HG13	2.19	0.42
1:B:46:LEU:O	1:B:50:THR:HG23	2.18	0.42
1:B:103:LEU:HD22	1:B:312:GLN:HG3	2.00	0.42
1:A:14:ASP:OD2	1:A:18:ARG:NH1	2.52	0.42
1:B:255:SER:O	1:B:259:ILE:HG13	2.19	0.42
1:B:300:ARG:HA	1:B:301:PRO:HD3	1.83	0.42
1:B:313:GLU:OE2	1:B:313:GLU:HA	2.20	0.42
1:A:209:ASN:HD22	1:A:209:ASN:HA	1.54	0.42
1:A:227:PRO:HA	1:A:234:SER:HB3	2.02	0.42
1:B:254:LEU:HD13	1:B:373:MET:CE	2.49	0.42
1:A:64:PHE:CG	1:A:71:MET:HE2	2.54	0.42
1:A:342:ILE:HD11	1:B:32:VAL:HG22	2.02	0.42
1:B:254:LEU:HD13	1:B:373:MET:HE2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ASN:HD22	1:B:209:ASN:HA	1.58	0.41
1:B:3:HIS:HA	1:B:4:PRO:HD2	1.90	0.41
1:B:64:PHE:CD1	1:B:71:MET:HE2	2.55	0.41
1:A:89:ASP:HA	1:A:145:LYS:NZ	2.36	0.41
1:B:356:ARG:HB2	1:B:356:ARG:NH1	2.36	0.41
1:A:20:PHE:CG	1:A:373:MET:HG2	2.56	0.41
1:A:45:MET:HE3	1:A:113:PHE:CZ	2.53	0.41
1:A:209:ASN:ND2	1:A:268:ARG:HG2	2.36	0.41
1:A:336:SER:O	1:A:337:SER:C	2.63	0.41
1:B:13:SER:O	1:B:17:VAL:HG23	2.21	0.41
1:A:94:THR:HG21	1:A:139:TRP:HE1	1.86	0.41
1:B:306:PHE:CZ	1:B:317:VAL:HG23	2.56	0.40
1:A:7:TYR:CD1	1:A:11:LEU:HG	2.55	0.40
1:A:363:ARG:HH11	1:A:363:ARG:HD2	1.60	0.40
1:B:181:ASP:O	1:B:182:SER:C	2.64	0.40
1:A:45:MET:HA	1:A:117:PHE:CZ	2.56	0.40
1:A:72:ALA:N	1:A:73:PRO:CD	2.85	0.40
1:B:4:PRO:HG2	1:B:7:TYR:CD2	2.52	0.40
1:B:45:MET:HA	1:B:117:PHE:CZ	2.56	0.40
1:A:122:LYS:HE3	1:A:139:TRP:CZ3	2.56	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	375/377 (100%)	350 (93%)	18 (5%)	7 (2%)	<b>6</b>   <b>17</b>
1	B	358/377 (95%)	342 (96%)	12 (3%)	4 (1%)	<b>11</b>   <b>29</b>
All	All	733/754 (97%)	692 (94%)	30 (4%)	11 (2%)	<b>8</b>   <b>22</b>

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	PRO
1	A	349	PRO
1	A	84	GLY
1	B	182	SER
1	B	191	LYS
1	A	4	PRO
1	A	313	GLU
1	A	338	SER
1	B	84	GLY
1	A	191	LYS
1	B	313	GLU

### 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	331/331 (100%)	294 (89%)	37 (11%)	<b>6</b> <b>15</b>
1	B	320/331 (97%)	289 (90%)	31 (10%)	<b>8</b> <b>20</b>
All	All	651/662 (98%)	583 (90%)	68 (10%)	<b>7</b> <b>17</b>

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	5	PRO
1	A	8	VAL
1	A	27	SER
1	A	43	LEU
1	A	82	LEU
1	A	92	SER
1	A	94	THR
1	A	101	ARG
1	A	106	VAL
1	A	107	GLN
1	A	110	MET
1	A	116	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	121	VAL
1	A	129	VAL
1	A	151	LEU
1	A	196	THR
1	A	209	ASN
1	A	224	LEU
1	A	231	ASP
1	A	244	GLU
1	A	257	GLN
1	A	258	LEU
1	A	261	HIS
1	A	272	LEU
1	A	273	LEU
1	A	303	GLN
1	A	312	GLN
1	A	313	GLU
1	A	315	LEU
1	A	331	SER
1	A	333	THR
1	A	336	SER
1	A	341	VAL
1	A	356	ARG
1	A	359	LEU
1	A	373	MET
1	B	7	TYR
1	B	8	VAL
1	B	27	SER
1	B	82	LEU
1	B	94	THR
1	B	101	ARG
1	B	103	LEU
1	B	106	VAL
1	B	107	GLN
1	B	110	MET
1	B	129	VAL
1	B	151	LEU
1	B	196	THR
1	B	204	GLN
1	B	209	ASN
1	B	224	LEU
1	B	244	GLU
1	B	251	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	257	GLN
1	B	258	LEU
1	B	261	HIS
1	B	267	THR
1	B	272	LEU
1	B	273	LEU
1	B	303	GLN
1	B	312	GLN
1	B	313	GLU
1	B	315	LEU
1	B	331	SER
1	B	356	ARG
1	B	359	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	22	GLN
1	A	47	GLN
1	A	55	GLN
1	A	59	GLN
1	A	100	GLN
1	A	167	ASN
1	A	172	ASN
1	A	174	GLN
1	A	206	ASN
1	A	209	ASN
1	A	219	HIS
1	A	257	GLN
1	A	261	HIS
1	A	292	ASN
1	A	316	HIS
1	B	22	GLN
1	B	25	GLN
1	B	47	GLN
1	B	55	GLN
1	B	59	GLN
1	B	100	GLN
1	B	167	ASN
1	B	172	ASN
1	B	174	GLN
1	B	204	GLN

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Mol	Chain	Res	Type
1	B	206	ASN
1	B	209	ASN
1	B	219	HIS
1	B	252	ASN
1	B	257	GLN
1	B	261	HIS
1	B	292	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 [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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	377/377 (100%)	-1.44	2 (0%) 87 86	12, 32, 65, 101	0
1	B	362/377 (96%)	-1.42	0 100 100	12, 33, 58, 86	0
All	All	739/754 (98%)	-1.43	2 (0%) 90 89	12, 32, 63, 101	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	PRO	2.3
1	A	3	HIS	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.