



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:49 PM GMT

PDB ID : 1DB2  
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 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 <http://wwpdb.org/ValidationPDFNotes.html>

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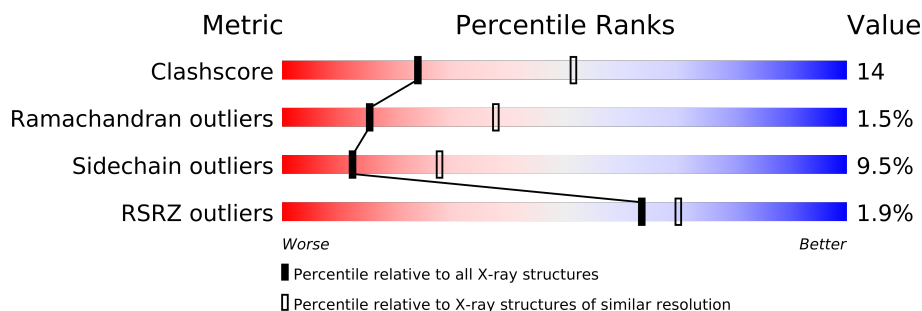
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	377	
1	B	377	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5887 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	A	377	Total	C	N	O	S	0	0	0
			2993	1921	510	547	15			
1	B	362	Total	C	N	O	S	0	0	0
			2894	1861	492	527	14			

There are 10 discrepancies between the modelled and reference sequences:

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

### 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.

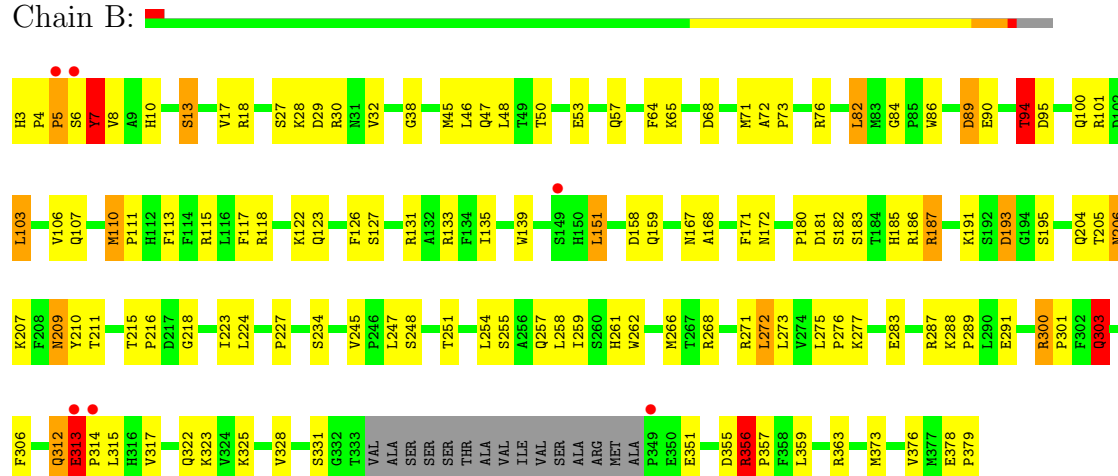
#### • Molecule 1: PLASMINOGEN ACTIVATOR INHIBITOR-1

Chain A:



#### • Molecule 1: PLASMINOGEN ACTIVATOR INHIBITOR-1

Chain B:



## 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 83.83 – 2.54	Depositor EDS
% Data completeness (in resolution range)	94.1 (20.00-2.70) 92.3 (83.83-2.54)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 2.55Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.255 , 0.299 0.208 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	35.3	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 1.2	EDS
Estimated twinning fraction	0.289 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 40258 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5887	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.78	5/3068 (0.2%)	1.45	27/4164 (0.6%)
1	B	0.69	2/2968 (0.1%)	1.48	32/4025 (0.8%)
All	All	0.74	7/6036 (0.1%)	1.46	59/8189 (0.7%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	HIS	C-N	10.95	1.55	1.34
1	A	379	PRO	C-OXT	6.79	1.36	1.23
1	B	379	PRO	C-O	6.71	1.36	1.23
1	B	379	PRO	C-OXT	6.28	1.35	1.23
1	A	3	HIS	CB-CG	6.21	1.61	1.50
1	A	379	PRO	C-O	6.14	1.35	1.23
1	A	3	HIS	CA-CB	5.43	1.65	1.53

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	18	ARG	NE-CZ-NH1	-16.32	112.14	120.30
1	B	133	ARG	NE-CZ-NH2	-15.64	112.48	120.30
1	A	187	ARG	NE-CZ-NH2	-13.47	113.56	120.30
1	B	30	ARG	NE-CZ-NH2	-10.36	115.12	120.30
1	B	18	ARG	NE-CZ-NH2	9.75	125.17	120.30
1	A	303	GLN	CA-CB-CG	9.33	133.92	113.40
1	B	5	PRO	CA-C-N	9.06	137.12	117.20
1	B	133	ARG	NE-CZ-NH1	8.73	124.66	120.30
1	A	133	ARG	NE-CZ-NH2	-8.69	115.96	120.30
1	A	115	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	B	95	ASP	CB-CG-OD2	-7.72	111.35	118.30
1	B	187	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	B	94	THR	N-CA-CB	7.25	124.08	110.30
1	B	115	ARG	NE-CZ-NH1	-7.23	116.68	120.30
1	B	158	ASP	CB-CG-OD2	6.98	124.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	THR	N-CA-CB	6.93	123.48	110.30
1	A	18	ARG	NE-CZ-NH2	6.79	123.69	120.30
1	B	271	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	3	HIS	CB-CA-C	6.74	123.87	110.40
1	A	300	ARG	NE-CZ-NH1	-6.72	116.94	120.30
1	B	303	GLN	CA-CB-CG	6.69	128.12	113.40
1	B	363	ARG	CD-NE-CZ	-6.68	114.24	123.60
1	A	5	PRO	O-C-N	-6.67	112.03	122.70
1	B	355	ASP	CB-CG-OD1	6.64	124.28	118.30
1	A	273	LEU	CA-CB-CG	6.58	130.44	115.30
1	A	287	ARG	CD-NE-CZ	6.42	132.59	123.60
1	A	359	LEU	CA-CB-CG	6.29	129.77	115.30
1	A	373	MET	CA-CB-CG	6.28	123.98	113.30
1	B	273	LEU	CA-CB-CG	6.23	129.63	115.30
1	A	69	LYS	CA-CB-CG	6.00	126.60	113.40
1	A	222	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	A	5	PRO	C-N-CA	5.97	136.63	121.70
1	B	10	HIS	CA-CB-CG	-5.87	103.62	113.60
1	B	356	ARG	NE-CZ-NH2	5.85	123.22	120.30
1	B	30	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	B	6	SER	N-CA-CB	5.73	119.10	110.50
1	A	5	PRO	CA-N-CD	-5.72	103.50	111.50
1	B	5	PRO	N-CA-C	5.70	126.91	112.10
1	A	131	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	B	6	SER	C-N-CA	5.60	135.71	121.70
1	B	378	GLU	C-N-CD	5.58	140.13	128.40
1	A	221	TYR	CA-CB-CG	5.58	124.00	113.40
1	A	303	GLN	N-CA-CB	-5.55	100.60	110.60
1	A	279	SER	N-CA-CB	-5.50	102.25	110.50
1	B	5	PRO	CA-C-O	-5.49	107.01	120.20
1	B	328	VAL	O-C-N	5.48	131.47	122.70
1	B	300	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	A	231	ASP	CB-CG-OD1	-5.36	113.48	118.30
1	B	218	GLY	N-CA-C	5.34	126.45	113.10
1	A	125	ASP	CB-CG-OD1	5.33	123.10	118.30
1	B	76	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	B	7	TYR	N-CA-CB	-5.29	101.07	110.60
1	B	68	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	218	GLY	N-CA-C	5.25	126.23	113.10
1	A	378	GLU	C-N-CD	5.24	139.41	128.40
1	A	301	PRO	N-CD-CG	-5.20	95.40	103.20
1	B	89	ASP	CB-CG-OD1	5.19	122.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	193	ASP	CB-CA-C	-5.08	100.24	110.40
1	A	4	PRO	CA-N-CD	-5.04	104.44	111.50

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2993	0	2987	82	0
1	B	2894	0	2880	89	0
All	All	5887	0	5867	167	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (167) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:B:206:ASN:ND2	1:B:207:LYS:H	1.75	0.84
1:A:206:ASN:HD22	1:A:207:LYS:N	1.76	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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: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:B:4:PRO:HG2	1:B:7:TYR:HD2	1.66	0.60
1:A:215:THR:HB	1:A:216:PRO:HD2	1.83	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:288:LYS:HB2	1:B:289:PRO:HD3	1.84	0.59
1:B:272:LEU:HD12	1:B:351:GLU:HG2	1.82	0.59
1:B:100:GLN:HE21	1:B:126:PHE:HB2	1.67	0.59
1:B:210:TYR:HD2	1:B:224:LEU:HD23	1.67	0.59
1:B:53:GLU:O	1:B:57:GLN:HG3	2.02	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:300:ARG:CB	1:B:303:GLN:HG3	2.34	0.57
1:B:101:ARG:HG2	1:B:123:GLN:HB3	1.86	0.57
1:B:47:GLN:HE22	1:B:65:LYS:HA	1.70	0.57
1:B:122:LYS:HE3	1:B:139:TRP:CH2	2.39	0.57
1:A:287:ARG:O	1:A:291:GLU:HG3	2.05	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:B:131:ARG:O	1:B:135:ILE:HG12	2.06	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:122:LYS:HD2	1:B:122:LYS:N	2.27	0.50
1:B:48:LEU:HD12	1:B:113:PHE:CD1	2.46	0.50
1:A:313:GLU:HA	1:A:313:GLU:OE2	2.11	0.50
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:206:ASN:ND2	1:A:207:LYS:N	2.49	0.48
1:B:45:MET:HE2	1:B:113:PHE:HZ	1.79	0.48
1:A:101:ARG:HB3	1:A:101:ARG:HH11	1.79	0.48
1:B:122:LYS:HE3	1:B:139:TRP:CZ3	2.48	0.48
1:A:305:ASP:OD1	1:A:307:THR:HG23	2.14	0.48
1:A:168:ALA:HA	1:A:323:LYS:O	2.14	0.48
1:B:64:PHE:CD1	1:B:71:MET:HE2	2.48	0.48
1:A:3:HIS:CD2	1:A:3:HIS:N	2.81	0.47
1:B:205:THR:HG22	1:B:272:LEU:HA	1.96	0.47
1:A:326:ILE:O	1:A:326:ILE:HG23	2.15	0.47
1:A:64:PHE:CD1	1:A:71:MET:HE2	2.49	0.47
1:A:110:MET:HA	1:A:110:MET:HE2	1.97	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:356:ARG:HB2	1:A:357:PRO:HD2	1.97	0.46
1:A:300:ARG:HA	1:A:301:PRO:HD3	1.55	0.46
1:A:230:GLY:O	1:A:231:ASP:HB2	2.15	0.46
1:B:117:PHE:O	1:B:118:ARG:HB2	2.16	0.46
1:A:301:PRO:HG3	1:A:316:HIS:CE1	2.51	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:300:ARG:HB2	1:B:303:GLN:HG3	1.98	0.45
1:A:254:LEU:HD13	1:A:373:MET:HE1	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:A:347:MET:HE2	1:B:325:LYS:HE3	1.99	0.45
1:A:87:ASN:CG	1:A:91:ILE:HG22	2.37	0.45
1:B:275:LEU:HA	1:B:276:PRO:HD3	1.88	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
1:B:110:MET:HA	1:B:110:MET:HE2	1.98	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:B:167:ASN:HD22	1:B:322:GLN:NE2	2.11	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:A:122:LYS:N	1:A:122:LYS:HD2	2.32	0.44
1:A:91:ILE:CD1	1:A:371:LEU:HD13	2.48	0.44
1:A:101:ARG:HB3	1:A:101:ARG:NH1	2.32	0.43
1:B:64:PHE:HB2	1:B:71:MET:HE2	2.00	0.43
1:B:90:GLU:O	1:B:171:PHE:HA	2.18	0.43
1:A:315:LEU:HA	1:A:315:LEU:HD23	1.90	0.43
1:A:90:GLU:O	1:A:171:PHE:HA	2.18	0.43
1:B:167:ASN:O	1:B:322:GLN:HA	2.18	0.43
1:A:313:GLU:HB3	1:A:314:PRO:HD3	2.00	0.43
1:B:356:ARG:HB2	1:B:357:PRO:HD2	2.00	0.43
1:B:211:THR:HG23	1:B:223:ILE:HD13	2.00	0.43
1:A:349:PRO:HG2	1:A:350:GLU:H	1.82	0.43
1:B:94:THR:HG21	1:B:139:TRP:HE1	1.82	0.43
1:B:247:LEU:HA	1:B:247:LEU:HD12	1.84	0.43
1:B:185:HIS:HD1	1:B:185:HIS:H	1.67	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: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:B:356:ARG:O	1:B:357:PRO:C	2.56	0.42
1:A:14:ASP:OD2	1:A:18:ARG:NH1	2.52	0.42
1:B:300:ARG:HA	1:B:301:PRO:HD3	1.83	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:255:SER:O	1:B:259:ILE:HG13	2.19	0.42
1:B:313:GLU:HA	1:B:313:GLU:OE2	2.20	0.42
1:A:227:PRO:HA	1:A:234:SER:HB3	2.02	0.42
1:A:209:ASN:HD22	1:A:209:ASN:HA	1.54	0.42
1:B:254:LEU:HD13	1:B:373:MET:CE	2.49	0.42
1:A:342:ILE:HD11	1:B:32:VAL:HG22	2.02	0.42
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:356:ARG:NH1	1:B:356:ARG:HB2	2.36	0.41
1:A:89:ASP:HA	1:A:145:LYS:NZ	2.36	0.41
1:A:20:PHE:CG	1:A:373:MET:HG2	2.56	0.41
1:A:209:ASN:ND2	1:A:268:ARG:HG2	2.36	0.41
1:A:165:LEU:HD12	1:A:165:LEU:C	2.41	0.41
1:B:376:VAL:O	1:B:376:VAL:HG12	2.21	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:B:64:PHE:CG	1:B:71:MET:HE2	2.56	0.40
1:A:363:ARG:HD2	1:A:363:ARG:HH11	1.60	0.40
1:B:4:PRO:HG2	1:B:7:TYR:CD2	2.52	0.40
1:A:72:ALA:N	1:A:73:PRO:CD	2.85	0.40
1:B:45:MET:HA	1:B:117:PHE:CZ	2.56	0.40
1:A:45:MET:HA	1:A: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

### 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	375/377 (100%)	350 (93%)	18 (5%)	7 (2%)	12	29
1	B	358/377 (95%)	342 (96%)	12 (3%)	4 (1%)	21	49
All	All	733/754 (97%)	692 (94%)	30 (4%)	11 (2%)	15	38

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 ⓘ

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%)	297 (90%)	34 (10%)	10	23
1	B	320/331 (97%)	292 (91%)	28 (9%)	14	32
All	All	651/662 (98%)	589 (90%)	62 (10%)	12	28

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	5	PRO
1	A	7	TYR
1	A	8	VAL
1	A	27	SER
1	A	43	LEU
1	A	82	LEU
1	A	89	ASP
1	A	92	SER
1	A	94	THR
1	A	106	VAL
1	A	107	GLN
1	A	110	MET

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Mol	Chain	Res	Type
1	A	129	VAL
1	A	151	LEU
1	A	206	ASN
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	336	SER
1	A	341	VAL
1	A	356	ARG
1	A	359	LEU
1	B	7	TYR
1	B	8	VAL
1	B	13	SER
1	B	27	SER
1	B	82	LEU
1	B	89	ASP
1	B	94	THR
1	B	103	LEU
1	B	106	VAL
1	B	107	GLN
1	B	110	MET
1	B	151	LEU
1	B	172	ASN
1	B	204	GLN
1	B	206	ASN
1	B	209	ASN
1	B	257	GLN
1	B	258	LEU
1	B	261	HIS
1	B	272	LEU
1	B	277	LYS

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Mol	Chain	Res	Type
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
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	257	GLN
1	A	261	HIS
1	A	292	ASN
1	B	22	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
1	B	206	ASN
1	B	209	ASN
1	B	229	HIS
1	B	257	GLN
1	B	261	HIS
1	B	292	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates 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

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%)	-0.01	8 (2%) 60 67	12, 32, 65, 101	0
1	B	362/377 (96%)	-0.17	6 (1%) 67 73	12, 33, 58, 86	0
All	All	739/754 (98%)	-0.09	14 (1%) 64 70	12, 32, 63, 101	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	HIS	11.5
1	A	336	SER	7.1
1	A	335	ALA	6.9
1	A	5	PRO	6.5
1	B	314	PRO	5.1
1	A	334	VAL	4.8
1	A	4	PRO	4.8
1	B	6	SER	4.1
1	B	349	PRO	3.5
1	B	5	PRO	3.0
1	B	313	GLU	2.4
1	A	333	THR	2.2
1	B	149	SER	2.2
1	A	7	TYR	2.1

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

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

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.