



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:31 PM UTC

PDB ID : 1BWD / pdb_00001bwd
Title : INOSAMINE-PHOSPHATE AMIDINOTRANSFERASE STRB1 FROM STREPTOMYCES GRISEUS
Authors : Fritsche, E.; Bergner, A.; Humm, A.; Piepersberg, W.; Huber, R.
Deposited on : 1998-09-23
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

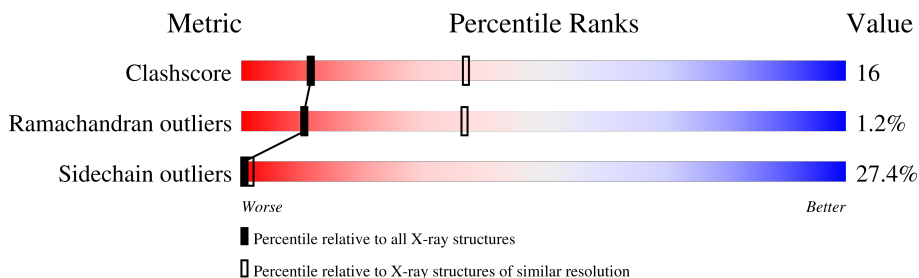
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

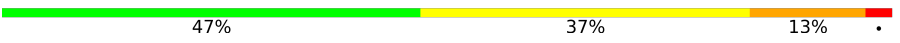
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)

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	348	 47% 37% 13% .
1	B	348	 45% 40% 11% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5455 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 PROTEIN (INOSAMINE-PHOSPHATE AMIDINOTRANSFERASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	19	0	0
			2728	1722	475	522	9			
1	B	348	Total	C	N	O	S	19	0	0
			2727	1722	475	521	9			

There are 6 discrepancies between the modelled and reference sequences:

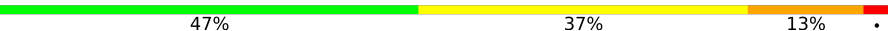
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ARG	MET	conflict	UNP P08078
A	341	GLY	-	insertion	UNP P08078
A	343	LEU	ARG	engineered mutation	UNP P08078
B	1	ARG	MET	conflict	UNP P08078
B	341	GLY	-	insertion	UNP P08078
B	343	LEU	ARG	engineered mutation	UNP P08078

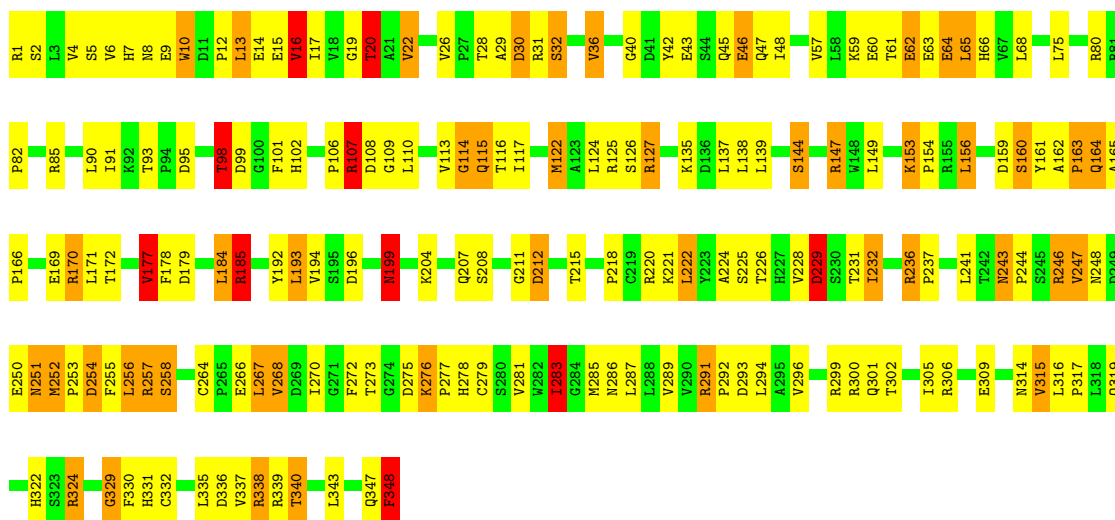
3 Residue-property plots

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.

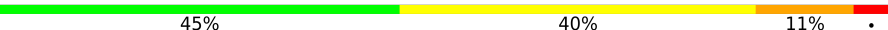
Note EDS was not executed.

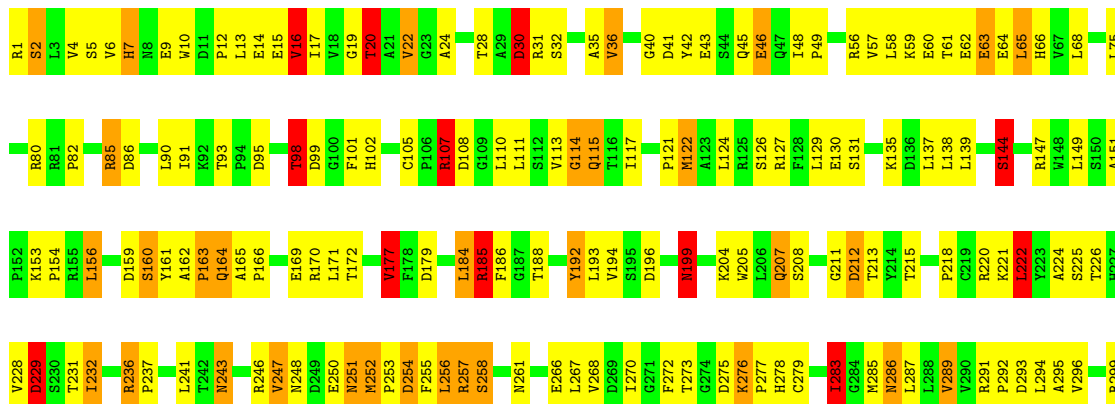
• Molecule 1: PROTEIN (INOSAMINE-PHOSPHATE AMIDINOTRANSFERASE)

Chain A: 



• Molecule 1: PROTEIN (INOSAMINE-PHOSPHATE AMIDINOTRANSFERASE)

Chain B: 



R300	Q301	T302	I305	R306	E309	V315	L316	P317	I318	Q319	H322	S323	R324	G329	F330	H331	C332	L335	D336	V337	R338	R339	T340	G341	I342	L343	Y346	Q347	F348
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	121.30Å 121.30Å 63.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.10	Depositor
% Data completeness (in resolution range)	86.0 (10.00-3.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.197 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5455	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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	1.04	4/2793 (0.1%)	1.93	70/3810 (1.8%)
1	B	1.06	3/2792 (0.1%)	1.89	69/3810 (1.8%)
All	All	1.05	7/5585 (0.1%)	1.91	139/7620 (1.8%)

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	1	0
1	B	1	0
All	All	2	0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	212	ASP	CA-CB	26.31	1.97	1.53
1	A	212	ASP	CA-CB	22.89	1.95	1.53
1	A	66	HIS	CA-CB	-22.09	1.18	1.53
1	B	159	ASP	CA-CB	-13.71	1.27	1.53
1	B	204	LYS	CA-CB	-12.67	1.33	1.53
1	A	204	LYS	CA-CB	-7.05	1.42	1.53
1	A	347	GLN	N-CA	5.28	1.53	1.46

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	ASP	CA-CB-CG	-25.84	86.76	112.60
1	B	159	ASP	CA-CB-CG	-15.89	96.70	112.60
1	B	185	ARG	CD-NE-CZ	14.84	145.17	124.40
1	A	212	ASP	CA-CB-CG	13.21	125.81	112.60
1	A	185	ARG	CD-NE-CZ	12.76	142.26	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	348	PHE	CA-CB-CG	10.96	124.75	113.80
1	B	212	ASP	CA-CB-CG	10.77	123.37	112.60
1	A	348	PHE	CA-CB-CG	10.76	124.56	113.80
1	A	159	ASP	CB-CA-C	10.24	131.92	110.32
1	A	278	HIS	CA-CB-CG	10.03	123.83	113.80
1	B	204	LYS	N-CA-CB	9.86	124.81	109.82
1	B	278	HIS	CA-CB-CG	9.69	123.49	113.80
1	B	246	ARG	CD-NE-CZ	9.56	137.79	124.40
1	A	212	ASP	N-CA-CB	-9.49	93.10	110.18
1	A	347	GLN	CA-C-O	-9.39	110.78	120.54
1	B	275	ASP	CA-C-O	9.14	133.58	120.51
1	A	246	ARG	CD-NE-CZ	9.04	137.06	124.40
1	A	108	ASP	N-CA-C	8.90	120.98	111.28
1	B	257	ARG	NE-CZ-NH1	-8.73	112.77	121.50
1	B	212	ASP	N-CA-CB	-8.57	96.60	110.14
1	A	7	HIS	CA-CB-CG	-8.49	105.31	113.80
1	A	22	VAL	CA-C-O	-8.48	110.18	120.78
1	B	179	ASP	CA-CB-CG	8.44	121.04	112.60
1	A	275	ASP	CA-C-O	8.40	132.53	120.51
1	B	108	ASP	N-CA-C	8.38	122.47	111.75
1	B	330	PHE	CA-CB-CG	-8.11	105.69	113.80
1	A	329	GLY	N-CA-C	-7.79	102.06	112.81
1	B	30	ASP	CA-CB-CG	7.79	120.39	112.60
1	A	20	THR	CB-CA-C	-7.76	97.02	110.45
1	B	22	VAL	CA-C-O	-7.63	111.24	120.78
1	B	16	VAL	CB-CA-C	-7.62	99.53	110.82
1	A	66	HIS	CA-CB-CG	7.54	121.33	113.80
1	A	16	VAL	CB-CA-C	-7.49	99.74	110.82
1	B	159	ASP	CB-CA-C	7.17	125.91	110.21
1	A	179	ASP	CA-CB-CG	7.15	119.75	112.60
1	A	338	ARG	CD-NE-CZ	7.07	134.29	124.40
1	B	257	ARG	NE-CZ-NH2	7.04	125.54	119.20
1	B	56	ARG	CA-C-O	-6.92	113.49	120.90
1	A	107	ARG	CA-C-N	6.90	129.53	120.28
1	A	107	ARG	C-N-CA	6.90	129.53	120.28
1	B	20	THR	CB-CA-C	-6.85	97.90	111.60
1	B	329	GLY	N-CA-C	-6.79	104.65	112.79
1	A	66	HIS	N-CA-CB	6.70	119.96	110.12
1	A	107	ARG	N-CA-C	6.69	118.58	111.28
1	A	204	LYS	CB-CA-C	-6.46	100.64	110.92
1	B	177	VAL	N-CA-CB	6.42	121.97	111.44
1	B	115	GLN	N-CA-C	-6.38	104.75	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	ARG	N-CA-C	6.34	119.11	108.02
1	A	330	PHE	CA-CB-CG	-6.33	107.47	113.80
1	B	7	HIS	CA-CB-CG	-6.33	107.47	113.80
1	B	98	THR	CB-CA-C	-6.32	99.27	111.78
1	A	30	ASP	CA-CB-CG	6.29	118.89	112.60
1	B	241	LEU	CA-C-O	-6.29	113.43	120.54
1	A	115	GLN	N-CA-C	-6.24	104.94	113.30
1	B	107	ARG	CA-C-N	6.21	129.45	120.38
1	B	107	ARG	C-N-CA	6.21	129.45	120.38
1	B	211	GLY	CA-C-N	6.18	129.40	120.38
1	B	211	GLY	C-N-CA	6.18	129.40	120.38
1	B	289	VAL	N-CA-CB	-6.15	104.07	110.95
1	A	127	ARG	NE-CZ-NH1	-6.10	115.40	121.50
1	A	159	ASP	N-CA-C	6.10	119.82	112.38
1	A	125	ARG	NE-CZ-NH2	6.03	124.63	119.20
1	B	121	PRO	CA-C-N	6.03	129.40	120.90
1	B	121	PRO	C-N-CA	6.03	129.40	120.90
1	A	32	SER	N-CA-C	5.93	117.41	111.07
1	B	66	HIS	CA-CB-CG	5.90	119.70	113.80
1	A	193	LEU	CA-C-O	-5.88	113.95	120.60
1	B	261	ASN	CA-CB-CG	5.88	118.48	112.60
1	A	276	LYS	CA-CB-CG	5.87	125.83	114.10
1	B	186	PHE	CA-CB-CG	5.86	119.66	113.80
1	A	243	ASN	CA-C-N	5.86	125.53	119.56
1	A	243	ASN	C-N-CA	5.86	125.53	119.56
1	B	302	THR	CA-C-O	-5.85	114.35	120.55
1	B	212	ASP	N-CA-C	5.85	119.24	111.75
1	B	207	GLN	N-CA-C	5.82	118.09	111.11
1	B	86	ASP	CA-C-O	-5.79	114.00	120.54
1	B	236	ARG	N-CA-C	-5.79	102.92	108.13
1	A	63	GLU	CA-CB-CG	5.78	125.66	114.10
1	A	178	PHE	CA-CB-CG	5.77	119.57	113.80
1	A	283	ILE	N-CA-CB	5.76	124.28	111.50
1	B	254	ASP	CA-CB-CG	-5.72	106.88	112.60
1	A	98	THR	CB-CA-C	-5.67	100.56	111.78
1	B	222	LEU	N-CA-C	-5.65	103.02	110.43
1	A	199	ASN	CA-CB-CG	5.64	118.24	112.60
1	B	276	LYS	CA-CB-CG	5.64	125.38	114.10
1	B	243	ASN	CA-C-N	5.63	125.25	119.56
1	B	243	ASN	C-N-CA	5.63	125.25	119.56
1	A	95	ASP	CA-CB-CG	-5.62	106.98	112.60
1	A	283	ILE	N-CA-C	-5.61	104.70	112.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	295	ALA	CA-C-N	-5.54	116.32	123.19
1	B	295	ALA	C-N-CA	-5.54	116.32	123.19
1	A	204	LYS	N-CA-CB	5.53	118.23	109.82
1	B	95	ASP	CA-CB-CG	-5.50	107.10	112.60
1	A	268	VAL	CB-CA-C	-5.50	103.54	111.34
1	B	63	GLU	CA-CB-CG	5.49	125.08	114.10
1	A	177	VAL	N-CA-CB	5.45	120.38	111.44
1	A	153	LYS	CA-C-N	5.43	125.34	119.85
1	A	153	LYS	C-N-CA	5.43	125.34	119.85
1	A	241	LEU	CA-C-O	-5.42	114.36	120.43
1	B	341	GLY	N-CA-C	5.41	118.20	110.46
1	A	185	ARG	N-CA-C	5.41	117.48	108.02
1	A	26	VAL	N-CA-C	-5.40	101.57	107.73
1	A	199	ASN	CA-C-N	5.39	127.50	120.28
1	A	199	ASN	C-N-CA	5.39	127.50	120.28
1	A	10	TRP	N-CA-CB	-5.39	103.84	111.00
1	B	270	ILE	O-C-N	-5.36	117.10	122.62
1	B	159	ASP	N-CA-C	5.35	119.29	112.87
1	B	346	TYR	N-CA-C	5.34	119.50	111.81
1	B	204	LYS	CB-CA-C	-5.33	102.45	110.92
1	A	127	ARG	NH1-CZ-NH2	5.31	126.20	119.30
1	A	62	GLU	CA-C-O	-5.30	114.80	120.42
1	B	199	ASN	CA-C-N	5.25	127.31	120.28
1	B	199	ASN	C-N-CA	5.25	127.31	120.28
1	A	291	ARG	N-CA-CB	5.24	116.60	111.10
1	A	254	ASP	CA-C-O	-5.23	114.87	120.42
1	B	283	ILE	N-CA-CB	5.21	121.98	111.05
1	A	13	LEU	N-CA-C	5.19	118.08	110.30
1	B	204	LYS	N-CA-C	-5.17	104.72	111.02
1	A	147	ARG	NE-CZ-NH1	-5.16	116.34	121.50
1	B	107	ARG	N-CA-C	5.14	116.89	111.28
1	B	147	ARG	NE-CZ-NH1	-5.14	116.36	121.50
1	A	64	GLU	CA-C-O	5.13	125.99	120.55
1	B	236	ARG	N-CA-CB	5.12	116.09	111.27
1	A	300	ARG	N-CA-C	-5.12	107.08	113.38
1	B	129	LEU	CA-C-N	5.11	127.44	120.54
1	B	129	LEU	C-N-CA	5.11	127.44	120.54
1	A	229	ASP	N-CA-CB	-5.10	101.87	110.49
1	A	270	ILE	CA-C-O	-5.08	116.99	121.97
1	A	163	PRO	CA-C-N	5.08	129.20	120.72
1	A	163	PRO	C-N-CA	5.08	129.20	120.72
1	A	257	ARG	CD-NE-CZ	-5.08	117.30	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ARG	CA-C-O	-5.07	115.09	121.02
1	B	41	ASP	N-CA-C	-5.06	107.76	114.04
1	A	236	ARG	N-CA-C	-5.06	103.58	108.13
1	A	211	GLY	CA-C-N	5.04	128.74	120.63
1	A	211	GLY	C-N-CA	5.04	128.74	120.63
1	B	229	ASP	N-CA-C	5.01	121.48	110.80
1	B	276	LYS	CB-CG-CD	5.00	122.81	111.30
1	B	229	ASP	N-CA-CB	-5.00	102.03	110.49

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	159	ASP	CA
1	B	159	ASP	CA

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	2728	0	2682	85	0
1	B	2727	0	2682	88	0
All	All	5455	0	5364	173	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 16.

All (173) 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:B:254:ASP:HA	1:B:257:ARG:HD2	1.58	0.82
1:A:283:ILE:HD11	1:A:324:ARG:HG2	1.62	0.81
1:A:12:PRO:HB2	1:A:340:THR:HG23	1.63	0.80
1:B:283:ILE:HD11	1:B:324:ARG:HG2	1.64	0.79
1:A:254:ASP:HA	1:A:257:ARG:HD2	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ASN:HB3	1:A:329:GLY:HA3	1.67	0.75
1:B:12:PRO:HB2	1:B:340:THR:HG23	1.69	0.75
1:B:286:ASN:HB3	1:B:329:GLY:HA3	1.73	0.70
1:B:6:VAL:HG23	1:B:339:ARG:HG3	1.75	0.69
1:A:6:VAL:HG23	1:A:339:ARG:HG3	1.74	0.68
1:A:177:VAL:H	1:A:199:ASN:HD21	1.41	0.68
1:A:13:LEU:HD21	1:A:16:VAL:HG22	1.75	0.67
1:B:20:THR:HG22	1:B:62:GLU:OE1	1.95	0.66
1:A:248:ASN:H	1:A:251:ASN:HB2	1.62	0.65
1:B:10:TRP:NE1	1:B:237:PRO:HD3	2.11	0.65
1:A:171:LEU:HD21	1:A:177:VAL:HG22	1.78	0.64
1:A:107:ARG:NH2	1:A:336:ASP:OD1	2.30	0.64
1:B:248:ASN:H	1:B:251:ASN:HB2	1.62	0.64
1:B:107:ARG:NH2	1:B:336:ASP:OD1	2.30	0.63
1:B:268:VAL:HB	1:B:301:GLN:HE22	1.63	0.62
1:A:283:ILE:HD13	1:A:283:ILE:H	1.64	0.62
1:B:32:SER:O	1:B:36:VAL:HG13	2.00	0.61
1:B:305:ILE:HG12	1:B:315:VAL:HG21	1.82	0.61
1:B:61:THR:HG23	1:B:322:HIS:HD2	1.64	0.61
1:B:305:ILE:HG23	1:B:315:VAL:HG11	1.81	0.61
1:B:28:THR:HG22	1:B:98:THR:HG22	1.82	0.60
1:A:28:THR:HG22	1:A:98:THR:HG22	1.83	0.60
1:A:61:THR:HG23	1:A:322:HIS:HD2	1.65	0.60
1:B:299:ARG:HB3	1:B:317:PRO:HB2	1.83	0.60
1:B:171:LEU:HD21	1:B:177:VAL:HG22	1.84	0.59
1:B:231:THR:HG22	1:B:232:ILE:HD12	1.84	0.58
1:A:305:ILE:HG12	1:A:315:VAL:HG21	1.86	0.58
1:A:14:GLU:OE1	1:A:338:ARG:HD2	2.04	0.58
1:B:4:VAL:O	1:B:115:GLN:HA	2.04	0.58
1:A:305:ILE:HG23	1:A:315:VAL:HG11	1.85	0.57
1:A:4:VAL:O	1:A:115:GLN:HA	2.05	0.57
1:A:32:SER:O	1:A:36:VAL:HG13	2.05	0.57
1:A:13:LEU:HD21	1:A:16:VAL:CG2	2.35	0.56
1:A:177:VAL:H	1:A:199:ASN:ND2	2.02	0.56
1:A:20:THR:HG22	1:A:62:GLU:OE1	2.05	0.56
1:A:268:VAL:HB	1:A:301:GLN:HE22	1.70	0.56
1:B:252:MET:HE2	1:B:253:PRO:HD2	1.87	0.56
1:A:196:ASP:HB2	1:A:225:SER:O	2.06	0.56
1:B:17:ILE:HD12	1:B:335:LEU:HD12	1.88	0.55
1:A:164:GLN:H	1:A:164:GLN:NE2	2.05	0.55
1:A:154:PRO:HB2	1:A:156:LEU:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:GLU:O	1:B:64:GLU:HG3	2.06	0.55
1:A:60:GLU:O	1:A:64:GLU:HG3	2.07	0.54
1:A:15:GLU:OE1	1:A:338:ARG:NH2	2.40	0.54
1:A:19:GLY:HA2	1:A:82:PRO:CG	2.38	0.54
1:B:236:ARG:HB2	1:B:237:PRO:HD2	1.89	0.54
1:A:247:VAL:HG21	1:A:252:MET:HE1	1.88	0.54
1:A:19:GLY:HA2	1:A:82:PRO:HG2	1.90	0.54
1:A:289:VAL:O	1:A:339:ARG:NH2	2.41	0.54
1:A:10:TRP:NE1	1:A:237:PRO:HD3	2.23	0.54
1:B:283:ILE:H	1:B:283:ILE:HD13	1.73	0.54
1:A:17:ILE:HD12	1:A:335:LEU:HD12	1.90	0.53
1:A:236:ARG:HB2	1:A:237:PRO:HD2	1.90	0.53
1:B:164:GLN:NE2	1:B:164:GLN:H	2.06	0.53
1:A:248:ASN:H	1:A:251:ASN:CB	2.22	0.53
1:B:122:MET:HG2	1:B:127:ARG:HB2	1.91	0.52
1:A:162:ALA:HB3	1:A:170:ARG:HA	1.90	0.52
1:A:268:VAL:HB	1:A:301:GLN:NE2	2.25	0.52
1:B:15:GLU:OE2	1:B:80:ARG:NH1	2.42	0.52
1:B:15:GLU:OE1	1:B:338:ARG:NH2	2.42	0.52
1:B:268:VAL:HB	1:B:301:GLN:NE2	2.24	0.52
1:A:5:SER:HA	1:A:114:GLY:O	2.11	0.51
1:A:184:LEU:HD13	1:A:228:VAL:HG13	1.92	0.51
1:A:193:LEU:HD21	1:A:224:ALA:HB3	1.93	0.51
1:B:185:ARG:HG3	1:B:185:ARG:HH11	1.75	0.51
1:B:19:GLY:HA2	1:B:82:PRO:CG	2.40	0.51
1:B:289:VAL:O	1:B:339:ARG:NH2	2.43	0.51
1:B:30:ASP:O	1:B:31:ARG:C	2.53	0.50
1:A:253:PRO:HG2	1:A:256:LEU:HD23	1.93	0.50
1:B:291:ARG:HG2	1:B:294:LEU:HB3	1.94	0.50
1:A:61:THR:O	1:A:65:LEU:HB2	2.11	0.50
1:A:272:PHE:CZ	1:A:277:PRO:HD3	2.46	0.50
1:A:165:ALA:HB1	1:A:166:PRO:HD2	1.94	0.50
1:A:299:ARG:HB3	1:A:317:PRO:HB2	1.94	0.49
1:B:248:ASN:H	1:B:251:ASN:CB	2.25	0.49
1:B:13:LEU:HD21	1:B:16:VAL:HG22	1.94	0.49
1:B:192:TYR:O	1:B:218:PRO:HA	2.10	0.49
1:A:61:THR:HG23	1:A:322:HIS:CD2	2.46	0.49
1:B:19:GLY:HA2	1:B:82:PRO:HG2	1.94	0.49
1:B:184:LEU:HD13	1:B:228:VAL:HG13	1.94	0.49
1:B:154:PRO:HB2	1:B:156:LEU:HD13	1.95	0.48
1:B:164:GLN:H	1:B:164:GLN:CD	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:GLN:H	1:A:164:GLN:CD	2.21	0.48
1:A:122:MET:HG2	1:A:127:ARG:HB2	1.95	0.48
1:B:272:PHE:CZ	1:B:277:PRO:HD3	2.48	0.48
1:B:253:PRO:HG2	1:B:256:LEU:HD23	1.96	0.48
1:B:61:THR:HG23	1:B:322:HIS:CD2	2.47	0.48
1:A:192:TYR:O	1:A:218:PRO:HA	2.13	0.47
1:B:7:HIS:CD2	1:B:343:LEU:HD12	2.49	0.47
1:A:291:ARG:HG2	1:A:294:LEU:HB3	1.96	0.47
1:B:2:SER:HA	1:B:144:SER:O	2.13	0.47
1:B:177:VAL:H	1:B:199:ASN:HD21	1.63	0.47
1:B:243:ASN:C	1:B:243:ASN:HD22	2.23	0.47
1:A:305:ILE:O	1:A:309:GLU:HG3	2.14	0.47
1:B:305:ILE:HG23	1:B:315:VAL:CG1	2.43	0.47
1:B:291:ARG:HB2	1:B:292:PRO:HD2	1.97	0.47
1:A:15:GLU:OE2	1:A:80:ARG:NH1	2.43	0.47
1:B:5:SER:O	1:B:338:ARG:HA	2.15	0.46
1:A:291:ARG:HG3	1:A:293:ASP:OD1	2.16	0.46
1:A:20:THR:HB	1:A:22:VAL:H	1.80	0.46
1:B:193:LEU:HD21	1:B:224:ALA:HB3	1.97	0.46
1:B:222:LEU:HD22	1:B:232:ILE:HD11	1.98	0.46
1:A:305:ILE:HG23	1:A:315:VAL:CG1	2.45	0.46
1:B:101:PHE:HB3	1:B:102:HIS:H	1.42	0.46
1:B:20:THR:HB	1:B:22:VAL:H	1.80	0.46
1:B:285:MET:HE2	1:B:285:MET:HB3	1.80	0.46
1:A:160:SER:HA	1:A:172:THR:OG1	2.15	0.46
1:A:264:CYS:SG	1:A:267:LEU:HD11	2.56	0.45
1:A:229:ASP:OD1	1:A:331:HIS:ND1	2.39	0.45
1:B:105:CYS:SG	1:B:332:CYS:HB3	2.57	0.45
1:A:45:GLN:HA	1:A:48:ILE:HD12	1.98	0.45
1:B:291:ARG:HG3	1:B:293:ASP:OD1	2.17	0.45
1:B:165:ALA:HB1	1:B:166:PRO:HD2	1.99	0.45
1:B:272:PHE:CD2	1:B:277:PRO:HB3	2.52	0.45
1:A:29:ALA:HB1	1:A:45:GLN:O	2.16	0.45
1:A:247:VAL:HA	1:A:251:ASN:OD1	2.16	0.45
1:A:252:MET:HE3	1:A:252:MET:HA	1.99	0.45
1:A:291:ARG:HB2	1:A:292:PRO:HD2	1.99	0.45
1:B:24:ALA:HB3	1:B:58:LEU:HD21	1.99	0.45
1:A:231:THR:HG22	1:A:232:ILE:HD12	1.99	0.45
1:A:46:GLU:H	1:A:46:GLU:HG2	1.58	0.44
1:A:294:LEU:HA	1:A:314:ASN:O	2.17	0.44
1:B:165:ALA:HB1	1:B:166:PRO:CD	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:ASP:HB2	1:B:225:SER:O	2.17	0.44
1:B:14:GLU:OE2	1:B:340:THR:HG22	2.16	0.44
1:A:106:PRO:HB2	1:A:335:LEU:HB2	1.99	0.44
1:B:85:ARG:NH2	1:B:130:GLU:O	2.47	0.44
1:B:5:SER:HA	1:B:114:GLY:O	2.17	0.44
1:B:13:LEU:HD21	1:B:16:VAL:CG2	2.47	0.44
1:A:287:LEU:C	1:A:287:LEU:HD12	2.43	0.44
1:A:14:GLU:OE2	1:A:340:THR:HG22	2.18	0.44
1:A:185:ARG:HG3	1:A:185:ARG:HH11	1.83	0.44
1:A:258:SER:OG	1:A:348:PHE:HB2	2.17	0.44
1:A:222:LEU:HD22	1:A:232:ILE:HD11	1.99	0.43
1:A:156:LEU:HG	1:A:161:TYR:OH	2.17	0.43
1:B:151:ALA:HA	1:B:205:TRP:CZ2	2.54	0.43
1:B:177:VAL:H	1:B:199:ASN:ND2	2.17	0.43
1:A:165:ALA:HB1	1:A:166:PRO:CD	2.47	0.43
1:A:101:PHE:HB3	1:A:102:HIS:H	1.50	0.43
1:A:65:LEU:HD12	1:A:65:LEU:HA	1.89	0.43
1:B:35:ALA:HB2	1:B:163:PRO:HG3	2.00	0.42
1:B:160:SER:HA	1:B:172:THR:OG1	2.19	0.42
1:B:42:TYR:CZ	1:B:49:PRO:HD3	2.54	0.42
1:A:109:GLY:HA3	1:A:122:MET:HE1	2.01	0.42
1:B:188:THR:HG23	1:B:213:THR:O	2.19	0.42
1:B:257:ARG:HH11	1:B:257:ARG:HD3	1.47	0.42
1:A:285:MET:HE2	1:A:285:MET:HB3	1.86	0.42
1:B:20:THR:HG22	1:B:62:GLU:CD	2.44	0.42
1:B:32:SER:HB3	1:B:161:TYR:CE2	2.55	0.42
1:B:305:ILE:O	1:B:309:GLU:HG3	2.19	0.42
1:B:46:GLU:H	1:B:46:GLU:HG2	1.66	0.42
1:A:243:ASN:HA	1:A:244:PRO:HD2	1.85	0.42
1:B:247:VAL:HA	1:B:251:ASN:OD1	2.20	0.41
1:B:229:ASP:OD1	1:B:331:HIS:ND1	2.41	0.41
1:B:45:GLN:HA	1:B:48:ILE:HD12	2.02	0.41
1:A:116:THR:HA	1:A:147:ARG:O	2.20	0.41
1:A:184:LEU:HD21	1:A:232:ILE:O	2.20	0.41
1:B:251:ASN:HD22	1:B:251:ASN:HA	1.68	0.41
1:A:42:TYR:HD1	1:A:47:GLN:HE21	1.68	0.41
1:B:162:ALA:O	1:B:163:PRO:C	2.63	0.41
1:B:258:SER:OG	1:B:348:PHE:HB2	2.20	0.41
1:A:8:ASN:HA	1:A:185:ARG:O	2.21	0.41
1:B:255:PHE:CE2	1:B:256:LEU:HD13	2.55	0.41
1:B:287:LEU:C	1:B:287:LEU:HD12	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:PHE:CE2	1:A:256:LEU:HD13	2.56	0.40
1:A:12:PRO:O	1:A:340:THR:HG23	2.21	0.40
1:B:65:LEU:HD12	1:B:65:LEU:HA	1.88	0.40
1:B:156:LEU:HG	1:B:161:TYR:OH	2.22	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	346/348 (99%)	304 (88%)	39 (11%)	3 (1%)	14	44
1	B	346/348 (99%)	308 (89%)	33 (10%)	5 (1%)	9	34
All	All	692/696 (99%)	612 (88%)	72 (10%)	8 (1%)	10	37

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	144	SER
1	A	144	SER
1	B	286	ASN
1	B	229	ASP
1	A	40	GLY
1	A	114	GLY
1	B	40	GLY
1	B	114	GLY

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	299/299 (100%)	218 (73%)	81 (27%)	0	2
1	B	299/299 (100%)	216 (72%)	83 (28%)	0	1
All	All	598/598 (100%)	434 (73%)	164 (27%)	0	1

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ARG
1	A	2	SER
1	A	9	GLU
1	A	16	VAL
1	A	20	THR
1	A	30	ASP
1	A	36	VAL
1	A	43	GLU
1	A	46	GLU
1	A	57	VAL
1	A	59	LYS
1	A	65	LEU
1	A	68	LEU
1	A	75	LEU
1	A	85	ARG
1	A	90	LEU
1	A	91	ILE
1	A	93	THR
1	A	98	THR
1	A	99	ASP
1	A	107	ARG
1	A	110	LEU
1	A	113	VAL
1	A	117	ILE
1	A	122	MET
1	A	124	LEU
1	A	126	SER
1	A	135	LYS
1	A	137	LEU
1	A	138	LEU
1	A	139	LEU
1	A	144	SER
1	A	149	LEU

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Mol	Chain	Res	Type
1	A	153	LYS
1	A	156	LEU
1	A	160	SER
1	A	163	PRO
1	A	164	GLN
1	A	169	GLU
1	A	170	ARG
1	A	177	VAL
1	A	184	LEU
1	A	185	ARG
1	A	194	VAL
1	A	199	ASN
1	A	207	GLN
1	A	208	SER
1	A	212	ASP
1	A	215	THR
1	A	220	ARG
1	A	221	LYS
1	A	222	LEU
1	A	226	THR
1	A	229	ASP
1	A	232	ILE
1	A	246	ARG
1	A	247	VAL
1	A	250	GLU
1	A	251	ASN
1	A	252	MET
1	A	256	LEU
1	A	258	SER
1	A	266	GLU
1	A	267	LEU
1	A	273	THR
1	A	276	LYS
1	A	279	CYS
1	A	281	VAL
1	A	283	ILE
1	A	296	VAL
1	A	302	THR
1	A	306	ARG
1	A	315	VAL
1	A	316	LEU
1	A	319	GLN

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Mol	Chain	Res	Type
1	A	324	ARG
1	A	332	CYS
1	A	337	VAL
1	A	340	THR
1	A	343	LEU
1	A	348	PHE
1	B	1	ARG
1	B	2	SER
1	B	9	GLU
1	B	16	VAL
1	B	20	THR
1	B	30	ASP
1	B	36	VAL
1	B	43	GLU
1	B	46	GLU
1	B	57	VAL
1	B	59	LYS
1	B	63	GLU
1	B	65	LEU
1	B	68	LEU
1	B	75	LEU
1	B	85	ARG
1	B	90	LEU
1	B	91	ILE
1	B	93	THR
1	B	98	THR
1	B	99	ASP
1	B	107	ARG
1	B	110	LEU
1	B	111	LEU
1	B	113	VAL
1	B	117	ILE
1	B	122	MET
1	B	124	LEU
1	B	126	SER
1	B	131	SER
1	B	135	LYS
1	B	137	LEU
1	B	138	LEU
1	B	139	LEU
1	B	144	SER
1	B	149	LEU

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Mol	Chain	Res	Type
1	B	153	LYS
1	B	156	LEU
1	B	160	SER
1	B	163	PRO
1	B	164	GLN
1	B	169	GLU
1	B	170	ARG
1	B	177	VAL
1	B	184	LEU
1	B	185	ARG
1	B	192	TYR
1	B	194	VAL
1	B	199	ASN
1	B	207	GLN
1	B	208	SER
1	B	212	ASP
1	B	215	THR
1	B	220	ARG
1	B	221	LYS
1	B	222	LEU
1	B	226	THR
1	B	229	ASP
1	B	232	ILE
1	B	247	VAL
1	B	250	GLU
1	B	251	ASN
1	B	252	MET
1	B	256	LEU
1	B	258	SER
1	B	266	GLU
1	B	267	LEU
1	B	273	THR
1	B	276	LYS
1	B	279	CYS
1	B	283	ILE
1	B	296	VAL
1	B	302	THR
1	B	306	ARG
1	B	315	VAL
1	B	316	LEU
1	B	319	GLN
1	B	324	ARG

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Mol	Chain	Res	Type
1	B	332	CYS
1	B	337	VAL
1	B	340	THR
1	B	343	LEU
1	B	348	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	HIS
1	A	47	GLN
1	A	164	GLN
1	A	199	ASN
1	A	243	ASN
1	B	7	HIS
1	B	45	GLN
1	B	47	GLN
1	B	164	GLN
1	B	199	ASN
1	B	243	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

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.