Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 06:40 PM GMT

PDB ID	:	1BWD
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.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

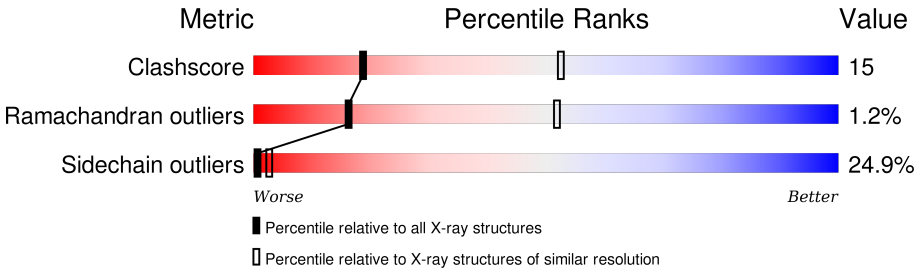
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	348	49% 39% 10%
1	B	348	50% 37% 11%

2 Entry composition (i)

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	UNP P08078
B	1	ARG	MET	CONFLICT	UNP P08078
B	341	GLY	-	INSERTION	UNP P08078
B	343	LEU	ARG	ENGINEERED	UNP P08078

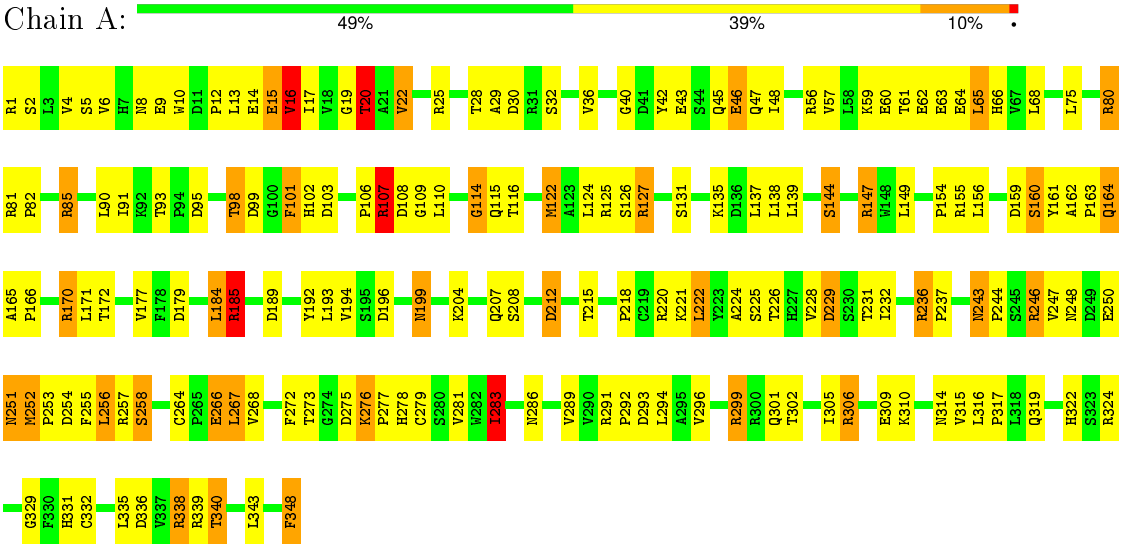
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

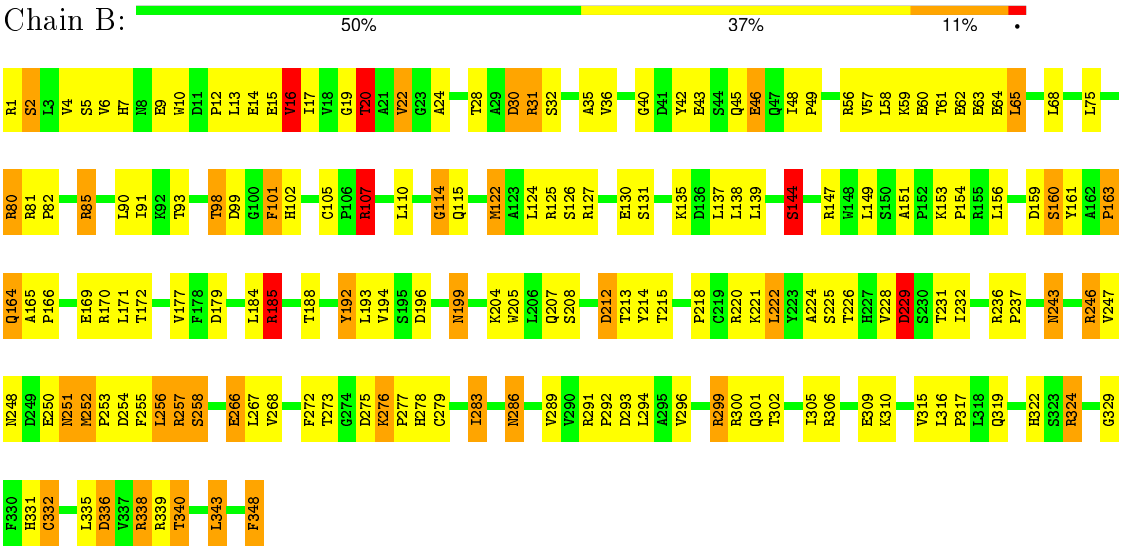
- Molecule 1: PROTEIN (INOSAMINE-PHOSPHATE AMIDINOTRANSFERASE)

Chain A:



- Molecule 1: PROTEIN (INOSAMINE-PHOSPHATE AMIDINOTRANSFERASE)

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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	0.82	3/2793 (0.1%)	1.54	44/3810 (1.2%)
1	B	0.84	3/2792 (0.1%)	1.52	33/3810 (0.9%)
All	All	0.83	6/5585 (0.1%)	1.53	77/7620 (1.0%)

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	1	0
1	B	1	0
All	All	2	0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	212	ASP	CA-CB	19.96	1.97	1.53
1	A	212	ASP	CA-CB	19.04	1.95	1.53
1	A	66	HIS	CA-CB	-15.96	1.18	1.53
1	B	159	ASP	CA-CB	-11.89	1.27	1.53
1	B	204	LYS	CA-CB	-9.31	1.33	1.53
1	A	204	LYS	CA-CB	-5.28	1.42	1.53

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	185	ARG	CD-NE-CZ	15.41	145.17	123.60
1	B	257	ARG	NE-CZ-NH1	-15.06	112.77	120.30
1	A	185	ARG	CD-NE-CZ	13.33	142.26	123.60
1	A	159	ASP	CA-CB-CG	-12.11	86.76	113.40
1	B	246	ARG	NE-CZ-NH1	11.67	126.14	120.30
1	A	185	ARG	NE-CZ-NH1	11.45	126.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	185	ARG	NE-CZ-NH2	-10.90	114.85	120.30
1	A	159	ASP	CB-CA-C	10.76	131.92	110.40
1	B	257	ARG	NE-CZ-NH2	10.48	125.54	120.30
1	B	246	ARG	CD-NE-CZ	10.13	137.79	123.60
1	B	299	ARG	NE-CZ-NH2	-9.92	115.34	120.30
1	A	127	ARG	NE-CZ-NH1	-9.81	115.40	120.30
1	A	212	ASP	N-CA-CB	-9.72	93.10	110.60
1	A	246	ARG	CD-NE-CZ	9.61	137.06	123.60
1	A	107	ARG	NE-CZ-NH2	-9.12	115.74	120.30
1	A	125	ARG	NE-CZ-NH2	8.66	124.63	120.30
1	B	80	ARG	NE-CZ-NH2	-8.57	116.02	120.30
1	B	107	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	A	246	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	B	246	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	B	338	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	A	147	ARG	NE-CZ-NH1	-7.92	116.34	120.30
1	B	204	LYS	N-CA-CB	7.89	124.81	110.60
1	B	147	ARG	NE-CZ-NH1	-7.88	116.36	120.30
1	B	81	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	B	212	ASP	N-CA-CB	-7.78	96.60	110.60
1	A	338	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	B	159	ASP	CB-CA-C	7.75	125.91	110.40
1	A	338	ARG	CD-NE-CZ	7.64	134.29	123.60
1	B	159	ASP	CA-CB-CG	-7.59	96.70	113.40
1	A	299	ARG	NE-CZ-NH2	-7.43	116.59	120.30
1	A	179	ASP	CB-CG-OD1	7.42	124.97	118.30
1	A	95	ASP	CB-CG-OD2	7.09	124.68	118.30
1	A	80	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	A	266	GLU	OE1-CD-OE2	6.92	131.61	123.30
1	B	266	GLU	OE1-CD-OE2	6.54	131.15	123.30
1	B	275	ASP	CA-C-O	6.42	133.58	120.10
1	B	179	ASP	CB-CG-OD1	6.36	124.03	118.30
1	A	56	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	A	236	ARG	NE-CZ-NH2	6.28	123.44	120.30
1	A	108	ASP	CB-CG-OD1	6.25	123.93	118.30
1	B	16	VAL	CB-CA-C	-6.25	99.53	111.40
1	A	127	ARG	NH1-CZ-NH2	6.18	126.20	119.40
1	A	16	VAL	CB-CA-C	-6.14	99.74	111.40
1	A	81	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	56	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	A	278	HIS	CA-CB-CG	6.02	123.83	113.60
1	B	22	VAL	CA-C-N	5.98	128.16	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	212	ASP	CB-CG-OD1	5.97	123.68	118.30
1	A	212	ASP	CB-CG-OD1	5.96	123.66	118.30
1	A	275	ASP	CA-C-O	5.92	132.53	120.10
1	B	214	TYR	CB-CG-CD2	-5.88	117.47	121.00
1	A	283	ILE	N-CA-CB	5.86	124.28	110.80
1	B	278	HIS	CA-CB-CG	5.82	123.49	113.60
1	A	15	GLU	OE1-CD-OE2	-5.81	116.33	123.30
1	A	22	VAL	CA-C-N	5.74	127.69	116.20
1	A	80	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	85	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	276	LYS	CA-CB-CG	5.65	125.83	113.40
1	B	336	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	212	ASP	CA-CB-CG	5.64	125.81	113.40
1	B	125	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	A	63	GLU	CA-CB-CG	5.57	125.66	113.40
1	A	25	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	A	155	ARG	CD-NE-CZ	5.45	131.22	123.60
1	B	276	LYS	CA-CB-CG	5.44	125.38	113.40
1	A	20	THR	CB-CA-C	-5.40	97.02	111.60
1	B	338	ARG	CD-NE-CZ	5.31	131.03	123.60
1	B	63	GLU	CA-CB-CG	5.31	125.08	113.40
1	B	80	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	A	189	ASP	CB-CG-OD1	5.25	123.02	118.30
1	A	66	HIS	N-CA-CB	5.20	119.96	110.60
1	B	300	ARG	NE-CZ-NH2	5.13	122.87	120.30
1	A	103	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	20	THR	CB-CA-C	-5.08	97.90	111.60
1	A	306	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	246	ARG	NE-CZ-NH2	-5.02	117.79	120.30

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 (i)

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	81	0
1	B	2727	0	2682	84	0
All	All	5455	0	5364	165	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 (165) 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
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:305:ILE:HG23	1:B:315:VAL:HG11	1.81	0.61
1:B:61:THR:HG23	1:B:322:HIS:HD2	1.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NE2	1:A:164:GLN:H	2.05	0.55
1:A:154:PRO:HB2	1:A:156:LEU:HD13	1.89	0.55
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:B:236:ARG:HB2	1:B:237:PRO:HD2	1.89	0.54
1:A:19:GLY:HA2	1:A:82:PRO:CG	2.38	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:H	1:B:164:GLN:NE2	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:268:VAL:HB	1:A:301:GLN:NE2	2.25	0.52
1:A:162:ALA:HB3	1:A:170:ARG:HA	1.90	0.52
1:A:252:MET:HE2	1:A:253:PRO:HD2	1.90	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:184:LEU:HD13	1:A:228:VAL:HG13	1.92	0.51
1:A:5:SER:HA	1:A:114:GLY:O	2.11	0.51
1:A:193:LEU:HD21	1:A:224:ALA:HB3	1.93	0.51
1:B:185:ARG:HH11	1:B:185:ARG:HG3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:305:ILE:HG23	1:B:315:VAL:CG1	2.43	0.47
1:A:305:ILE:O	1:A:309:GLU:HG3	2.14	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:B:222:LEU:HD22	1:B:232:ILE:HD11	1.98	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: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:30:ASP:O	1:B:31:ARG:C	2.53	0.46
1:B:20:THR:HB	1:B:22:VAL:H	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:B:105:CYS:SG	1:B:332:CYS:HB3	2.57	0.45
1:A:229:ASP:OD1	1:A:331:HIS:ND1	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:ARG:HG3	1:B:293:ASP:OD1	2.17	0.45
1:A:45:GLN:HA	1:A:48:ILE:HD12	1.98	0.45
1:B:272:PHE:CD2	1:B:277:PRO:HB3	2.52	0.45
1:B:165:ALA:HB1	1:B:166:PRO:HD2	1.99	0.45
1:A:247:VAL:HA	1:A:251:ASN:OD1	2.16	0.45
1:A:291:ARG:HB2	1:A:292:PRO:HD2	1.99	0.45
1:A:29:ALA:HB1	1:A:45:GLN:O	2.16	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: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
1:B:196:ASP:HB2	1:B:225:SER:O	2.17	0.44
1:A:46:GLU:HG2	1:A:46:GLU:H	1.58	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:A:109:GLY:HA3	1:A:122:MET:HE1	1.99	0.44
1:B:13:LEU:HD21	1:B:16:VAL:CG2	2.47	0.44
1:B:164:GLN:CD	1:B:164:GLN:H	2.21	0.44
1:A:14:GLU:OE2	1:A:340:THR:HG22	2.18	0.44
1:A:258:SER:OG	1:A:348:PHE:HB2	2.17	0.44
1:A:185:ARG:HH11	1:A:185:ARG:HG3	1.83	0.44
1:A:222:LEU:HD22	1:A:232:ILE:HD11	1.99	0.43
1:B:177:VAL:H	1:B:199:ASN:ND2	2.17	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: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:HA	1:A:65:LEU:HD12	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: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:B:243:ASN:C	1:B:243:ASN:HD22	2.23	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:HG2	1:B:46:GLU:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:251:ASN:HA	1:B:251:ASN:HD22	1.68	0.41
1:A:184:LEU:HD21	1:A:232:ILE:O	2.20	0.41
1:A:116:THR:HA	1:A:147:ARG:O	2.20	0.41
1:B:258:SER:OG	1:B:348:PHE:HB2	2.20	0.41
1:A:42:TYR:HD1	1:A:47:GLN:HE21	1.68	0.41
1:B:255:PHE:CE2	1:B:256:LEU:HD13	2.55	0.41
1:A:8:ASN:HA	1:A:185:ARG:O	2.21	0.41
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:156:LEU:HG	1:B:161:TYR:OH	2.22	0.40
1:B:65:LEU:HD12	1:B:65:LEU:HA	1.88	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%)	21	61
1	B	346/348 (99%)	308 (89%)	33 (10%)	5 (1%)	14	48
All	All	692/696 (99%)	612 (88%)	72 (10%)	8 (1%)	16	52

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

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Mol	Chain	Res	Type
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%)	226 (76%)	73 (24%)	1 3
1	B	299/299 (100%)	223 (75%)	76 (25%)	1 2
All	All	598/598 (100%)	449 (75%)	149 (25%)	1 3

All (149) 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	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	101	PHE

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Mol	Chain	Res	Type
1	A	107	ARG
1	A	110	LEU
1	A	122	MET
1	A	124	LEU
1	A	126	SER
1	A	131	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
1	A	160	SER
1	A	163	PRO
1	A	164	GLN
1	A	170	ARG
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	243	ASN
1	A	246	ARG
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

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Mol	Chain	Res	Type
1	A	283	ILE
1	A	296	VAL
1	A	302	THR
1	A	306	ARG
1	A	310	LYS
1	A	316	LEU
1	A	319	GLN
1	A	332	CYS
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	31	ARG
1	B	43	GLU
1	B	46	GLU
1	B	57	VAL
1	B	59	LYS
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	101	PHE
1	B	107	ARG
1	B	110	LEU
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

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Mol	Chain	Res	Type
1	B	144	SER
1	B	149	LEU
1	B	153	LYS
1	B	160	SER
1	B	163	PRO
1	B	164	GLN
1	B	169	GLU
1	B	170	ARG
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	243	ASN
1	B	246	ARG
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	310	LYS
1	B	316	LEU
1	B	319	GLN
1	B	324	ARG
1	B	332	CYS

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Mol	Chain	Res	Type
1	B	340	THR
1	B	343	LEU
1	B	348	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) 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	47	GLN
1	B	164	GLN
1	B	199	ASN
1	B	243	ASN

5.3.3 RNA

There are no RNA molecules 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

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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