Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:21 PM GMT

PDB ID	:	1TAB
Title	:	STRUCTURE OF THE TRYPSIN-BINDING DOMAIN OF BOWMAN-BIRK TYPE PROTEASE INHIBITOR AND ITS INTERACTION WITH TRYPSIN
Authors	:	Tsunogae, Y.; Tanaka, I.; Yamane, T.; Kikkawa, J.-I.; Ashida, T.; Ishikawa, C.; Watanabe, K.; Nakamura, S.; Takahashi, K.
Deposited on	:	1990-10-15
Resolution	:	2.30 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 (i) symbol.

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

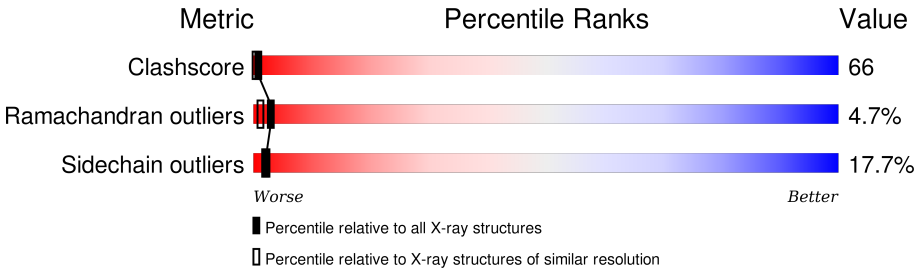
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.30 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	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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	E	223	31% 44% 20% 5%
2	I	82	. 13% 13% 13% 56%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2044 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 TRYPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			

- Molecule 2 is a protein called BOWMAN-BIRK TYPE PROTEINASE INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	36	Total	C	N	O	S	0	0	0
			275	162	48	56	9			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	136	Total	O	0	0
			136	136		
3	I	4	Total	O	0	0
			4	4		

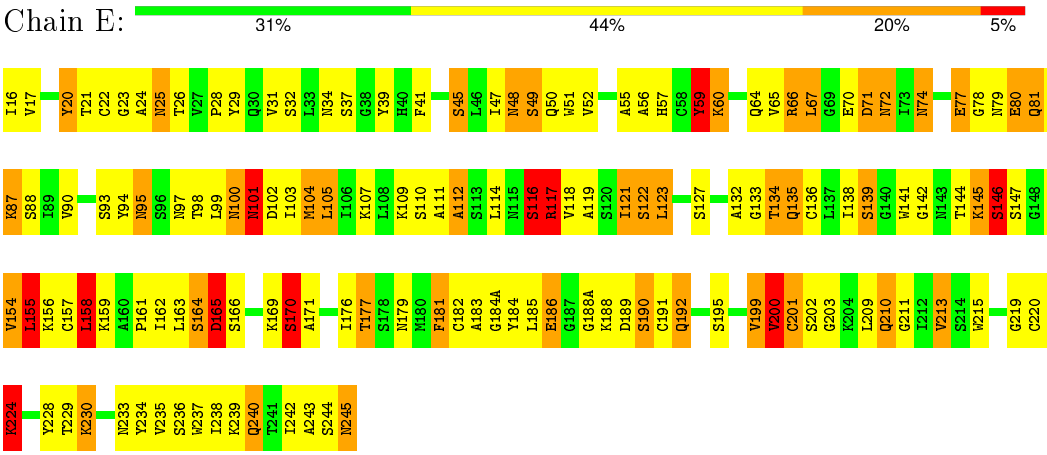
3 Residue-property plots (i)

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.

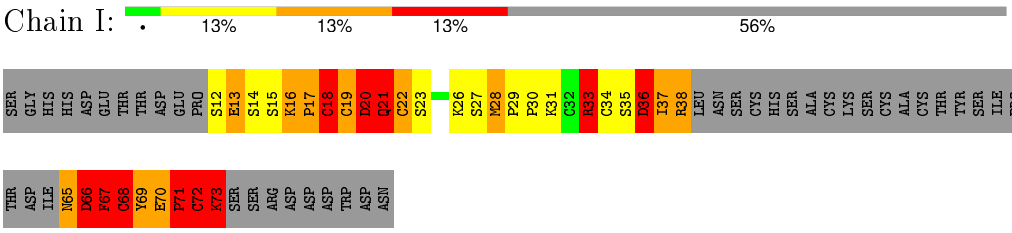
- Molecule 1: TRYPSIN

Chain E:



- Molecule 2: BOWMAN-BIRK TYPE PROTEINASE INHIBITOR

Chain I:



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 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	55.42Å 55.42Å 181.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.200 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2044	wwPDB-VP
Average B, all atoms (Å^2)	12.0	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	E	1.36	3/1660 (0.2%)	2.26	82/2250 (3.6%)
2	I	1.64	5/279 (1.8%)	3.62	48/371 (12.9%)
All	All	1.41	8/1939 (0.4%)	2.50	130/2621 (5.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	88	SER	CB-OG	-7.71	1.32	1.42
2	I	66	ASP	N-CA	-6.78	1.32	1.46
2	I	72	CYS	N-CA	-6.71	1.32	1.46
2	I	71	PRO	CA-CB	6.65	1.66	1.53
2	I	72	CYS	CB-SG	5.34	1.91	1.82
1	E	80	GLU	CD-OE1	-5.03	1.20	1.25
2	I	67	PHE	N-CA	-5.02	1.36	1.46
1	E	190	SER	CA-CB	-5.02	1.45	1.52

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	66	ARG	NE-CZ-NH1	21.06	130.83	120.30
2	I	65	ASN	C-N-CA	18.41	167.72	121.70
2	I	71	PRO	C-N-CA	17.82	166.25	121.70
2	I	65	ASN	CA-CB-CG	16.52	149.73	113.40
2	I	38	ARG	NE-CZ-NH1	14.72	127.66	120.30
2	I	66	ASP	C-N-CA	11.32	149.99	121.70
1	E	94	TYR	CB-CG-CD2	-11.08	114.35	121.00
1	E	111	ALA	N-CA-CB	10.79	125.20	110.10
2	I	22	CYS	N-CA-CB	10.57	129.63	110.60
1	E	101	ASN	CB-CG-OD1	10.42	142.43	121.60
1	E	151	TYR	CB-CG-CD2	10.32	127.19	121.00
1	E	151	TYR	CB-CG-CD1	-10.19	114.89	121.00
2	I	20	ASP	CB-CG-OD1	9.91	127.22	118.30
1	E	105	LEU	CB-CA-C	9.65	128.53	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	66	ASP	CA-C-O	9.18	139.37	120.10
1	E	158	LEU	CA-CB-CG	9.00	136.01	115.30
2	I	71	PRO	N-CA-C	8.65	134.59	112.10
2	I	20	ASP	CB-CG-OD2	-8.63	110.53	118.30
2	I	19	CYS	N-CA-CB	8.54	125.97	110.60
1	E	97	ASN	CA-CB-CG	8.26	131.57	113.40
1	E	94	TYR	CB-CG-CD1	8.26	125.95	121.00
1	E	245	ASN	CA-CB-CG	8.19	131.43	113.40
1	E	151	TYR	N-CA-CB	-8.01	96.19	110.60
2	I	66	ASP	N-CA-C	7.96	132.51	111.00
2	I	65	ASN	O-C-N	-7.85	110.14	122.70
1	E	66	ARG	NH1-CZ-NH2	-7.81	110.81	119.40
2	I	67	PHE	N-CA-CB	7.80	124.64	110.60
2	I	66	ASP	CB-CG-OD1	7.68	125.21	118.30
1	E	199	VAL	CA-CB-CG2	7.65	122.37	110.90
2	I	71	PRO	O-C-N	-7.51	110.69	122.70
1	E	105	LEU	N-CA-CB	-7.35	95.69	110.40
2	I	68	CYS	CB-CA-C	7.27	124.93	110.40
1	E	165	ASP	CB-CG-OD1	7.17	124.75	118.30
1	E	171	ALA	C-N-CA	7.14	139.56	121.70
2	I	38	ARG	CD-NE-CZ	7.07	133.50	123.60
2	I	20	ASP	CA-C-N	-6.86	102.10	117.20
2	I	68	CYS	CA-C-N	6.84	132.25	117.20
2	I	69	TYR	C-N-CA	6.82	138.74	121.70
2	I	72	CYS	CA-CB-SG	-6.81	101.74	114.00
2	I	72	CYS	N-CA-CB	6.68	122.62	110.60
2	I	18	CYS	C-N-CA	6.63	138.29	121.70
1	E	240	GLN	CG-CD-OE1	6.58	134.77	121.60
2	I	67	PHE	CB-CG-CD1	-6.57	116.20	120.80
1	E	150	SER	C-N-CA	6.57	138.12	121.70
2	I	36	ASP	CB-CG-OD2	6.54	124.19	118.30
2	I	31	LYS	CB-CA-C	6.53	123.45	110.40
1	E	81	GLN	CA-CB-CG	6.51	127.72	113.40
1	E	97	ASN	N-CA-CB	6.45	122.22	110.60
1	E	190	SER	CB-CA-C	6.43	122.31	110.10
2	I	38	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	E	60	LYS	CA-CB-CG	6.37	127.42	113.40
1	E	199	VAL	N-CA-CB	6.29	125.35	111.50
2	I	69	TYR	CA-C-O	6.29	133.31	120.10
1	E	101	ASN	OD1-CG-ND2	-6.24	107.56	121.90
1	E	102	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	E	186	GLU	OE1-CD-OE2	6.18	130.72	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	183	ALA	N-CA-CB	6.18	118.75	110.10
1	E	95	ASN	N-CA-CB	-6.13	99.56	110.60
1	E	181	PHE	CA-CB-CG	6.13	128.61	113.90
1	E	186	GLU	CG-CD-OE2	-6.11	106.09	118.30
1	E	101	ASN	CA-CB-CG	6.01	126.62	113.40
1	E	171	ALA	CB-CA-C	-6.00	101.10	110.10
2	I	67	PHE	C-N-CA	5.99	136.66	121.70
1	E	60	LYS	N-CA-CB	5.97	121.35	110.60
1	E	185	LEU	CA-CB-CG	5.94	128.95	115.30
1	E	200	VAL	CB-CA-C	5.93	122.67	111.40
1	E	59	TYR	C-N-CA	5.92	136.51	121.70
2	I	21	GLN	N-CA-CB	5.91	121.25	110.60
1	E	20	TYR	CB-CG-CD2	5.82	124.49	121.00
2	I	71	PRO	CA-C-O	5.79	134.10	120.20
2	I	19	CYS	CA-C-N	-5.76	104.53	117.20
1	E	230	LYS	CA-CB-CG	5.75	126.04	113.40
1	E	127	SER	CB-CA-C	5.74	121.00	110.10
1	E	81	GLN	N-CA-CB	5.73	120.92	110.60
1	E	117	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	E	146	SER	CA-CB-OG	5.69	126.56	111.20
2	I	71	PRO	N-CA-CB	-5.68	96.36	102.60
1	E	170	SER	CA-CB-OG	-5.67	95.88	111.20
1	E	20	TYR	CB-CG-CD1	-5.67	117.60	121.00
1	E	100	ASN	CB-CA-C	5.66	121.72	110.40
2	I	38	ARG	CA-CB-CG	5.65	125.82	113.40
1	E	184	TYR	CB-CG-CD2	-5.62	117.62	121.00
1	E	150	SER	N-CA-CB	5.59	118.88	110.50
1	E	170	SER	N-CA-CB	-5.59	102.12	110.50
1	E	103	ILE	C-N-CA	5.57	135.62	121.70
2	I	68	CYS	O-C-N	-5.54	113.84	122.70
1	E	165	ASP	OD1-CG-OD2	-5.53	112.80	123.30
1	E	111	ALA	N-CA-C	-5.52	96.10	111.00
1	E	230	LYS	N-CA-CB	5.51	120.51	110.60
2	I	72	CYS	C-N-CA	5.45	135.33	121.70
1	E	122	SER	O-C-N	5.45	131.42	122.70
1	E	80	GLU	CG-CD-OE1	5.43	129.16	118.30
1	E	184	TYR	CB-CG-CD1	5.43	124.26	121.00
1	E	109	LYS	C-N-CA	5.42	135.25	121.70
2	I	20	ASP	N-CA-CB	5.41	120.33	110.60
1	E	100	ASN	C-N-CA	5.40	135.21	121.70
1	E	154	VAL	CA-CB-CG2	5.39	118.98	110.90
2	I	20	ASP	CA-C-O	5.38	131.39	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	134	THR	CA-CB-CG2	5.33	119.86	112.40
2	I	66	ASP	CA-C-N	-5.33	105.48	117.20
2	I	18	CYS	CB-CA-C	5.33	121.05	110.40
1	E	86	SER	O-C-N	-5.31	114.20	122.70
1	E	77	GLU	CG-CD-OE2	-5.30	107.70	118.30
2	I	73	LYS	N-CA-CB	5.29	120.11	110.60
1	E	88	SER	N-CA-CB	-5.28	102.58	110.50
1	E	71	ASP	CB-CG-OD1	5.25	123.03	118.30
2	I	13	GLU	C-N-CA	5.22	134.75	121.70
1	E	157	CYS	CA-CB-SG	5.22	123.39	114.00
1	E	213	VAL	O-C-N	5.21	131.04	122.70
1	E	116	SER	O-C-N	5.21	131.03	122.70
1	E	112	ALA	CB-CA-C	5.20	117.91	110.10
2	I	33	ARG	CA-C-O	-5.20	109.18	120.10
1	E	111	ALA	CB-CA-C	5.19	117.89	110.10
1	E	185	LEU	CB-CA-C	5.17	120.02	110.20
2	I	36	ASP	CA-CB-CG	5.17	124.77	113.40
2	I	69	TYR	N-CA-C	5.17	124.95	111.00
2	I	21	GLN	O-C-N	5.14	130.93	122.70
1	E	104	MET	CA-CB-CG	-5.13	104.58	113.30
1	E	72	ASN	O-C-N	5.12	130.89	122.70
1	E	230	LYS	O-C-N	5.11	130.88	122.70
2	I	31	LYS	N-CA-C	-5.10	97.23	111.00
1	E	87	LYS	CB-CG-CD	5.10	124.86	111.60
1	E	155	LEU	CA-CB-CG	5.10	127.02	115.30
1	E	146	SER	N-CA-CB	5.09	118.14	110.50
1	E	139	SER	N-CA-CB	-5.09	102.87	110.50
1	E	105	LEU	CA-CB-CG	5.09	127.00	115.30
1	E	67	LEU	CB-CA-C	5.08	119.85	110.20
1	E	224	LYS	N-CA-CB	-5.06	101.48	110.60
1	E	142	GLY	C-N-CA	5.03	134.27	121.70
1	E	230	LYS	CG-CD-CE	5.01	126.93	111.90

There are no chirality outliers.

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	E	1629	0	1585	180	4
2	I	275	0	246	70	0
3	E	136	0	0	32	4
3	I	4	0	0	0	0
All	All	2044	0	1831	246	5

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 66.

All (246) 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)
2:I:13:GLU:HG3	2:I:14:SER:H	1.08	1.17
1:E:87:LYS:HE3	3:E:332:HOH:O	1.48	1.14
2:I:12:SER:HA	2:I:16:LYS:HD3	1.31	1.10
1:E:149:THR:HG23	1:E:151:TYR:CE2	1.89	1.07
2:I:17:PRO:O	2:I:20:ASP:HB2	1.57	1.05
1:E:135:GLN:HE21	1:E:159:LYS:HB3	1.17	1.04
2:I:36:ASP:O	2:I:37:ILE:HB	1.24	0.99
1:E:121:ILE:HD12	1:E:122:SER:H	1.25	0.98
1:E:149:THR:HG23	1:E:151:TYR:HE2	1.26	0.98
1:E:87:LYS:NZ	1:E:245:ASN:OD1	1.96	0.97
2:I:13:GLU:CG	2:I:14:SER:H	1.56	0.97
2:I:17:PRO:O	2:I:18:CYS:C	2.04	0.96
1:E:220:CYS:N	3:E:303:HOH:O	1.94	0.95
2:I:13:GLU:CG	2:I:14:SER:N	2.26	0.95
2:I:28:MET:CE	2:I:29:PRO:HA	1.95	0.94
2:I:33:ARG:HH11	2:I:33:ARG:HG3	1.31	0.94
2:I:72:CYS:SG	2:I:73:LYS:N	2.36	0.94
3:E:256:HOH:O	2:I:26:LYS:HE3	1.69	0.93
1:E:48:ASN:HD22	1:E:49:SER:N	1.65	0.93
2:I:36:ASP:O	2:I:37:ILE:CB	2.15	0.93
1:E:164:SER:HB3	1:E:166:SER:OG	1.69	0.93
2:I:13:GLU:HG3	2:I:14:SER:N	1.83	0.92
1:E:55:ALA:O	1:E:104:MET:HE2	1.71	0.90
2:I:17:PRO:O	2:I:18:CYS:O	1.90	0.89
1:E:55:ALA:O	1:E:104:MET:CE	2.22	0.88
1:E:135:GLN:NE2	1:E:159:LYS:HB3	1.87	0.88
2:I:21:GLN:O	2:I:34:CYS:HA	1.75	0.86
1:E:224:LYS:N	1:E:224:LYS:HD2	1.91	0.85
1:E:25:ASN:CG	1:E:117:ARG:HB3	1.96	0.85
2:I:12:SER:HA	2:I:16:LYS:CD	2.07	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:192:GLN:HG3	3:E:247:HOH:O	1.78	0.84
2:I:28:MET:HE2	2:I:29:PRO:HA	1.59	0.83
1:E:25:ASN:HA	3:E:260:HOH:O	1.78	0.83
2:I:67:PHE:O	2:I:68:CYS:SG	2.37	0.82
2:I:28:MET:HA	2:I:28:MET:HE2	1.59	0.82
1:E:25:ASN:ND2	1:E:117:ARG:HA	1.94	0.82
1:E:31:VAL:CG1	1:E:65:VAL:HG13	2.09	0.81
1:E:238:ILE:HG23	1:E:242:ILE:CD1	2.10	0.81
2:I:19:CYS:HA	2:I:36:ASP:OD1	1.80	0.81
2:I:18:CYS:O	2:I:69:TYR:HE2	1.64	0.80
2:I:28:MET:HE1	2:I:29:PRO:HA	1.62	0.80
1:E:80:GLU:HB3	1:E:82:PHE:CE2	2.17	0.80
1:E:25:ASN:CB	1:E:117:ARG:HB3	2.12	0.80
2:I:21:GLN:HA	2:I:21:GLN:OE1	1.73	0.79
1:E:119:ALA:HB2	3:E:372:HOH:O	1.83	0.79
2:I:67:PHE:C	2:I:68:CYS:SG	2.60	0.78
1:E:146:SER:OG	3:E:305:HOH:O	2.02	0.78
1:E:67:LEU:O	1:E:80:GLU:HA	1.83	0.78
1:E:105:LEU:HD11	1:E:242:ILE:HD11	1.67	0.77
1:E:223:ASN:C	1:E:224:LYS:HD2	2.06	0.76
1:E:121:ILE:HG21	1:E:209:LEU:HD22	1.67	0.76
1:E:121:ILE:HD12	1:E:122:SER:N	1.98	0.76
1:E:31:VAL:HG22	1:E:67:LEU:HD23	1.67	0.75
1:E:83:ILE:HG21	1:E:110:SER:HB2	1.69	0.74
1:E:79:ASN:O	3:E:333:HOH:O	2.05	0.74
1:E:93:SER:HB2	1:E:101:ASN:HD21	1.53	0.73
2:I:37:ILE:O	2:I:38:ARG:HG2	1.89	0.72
1:E:87:LYS:HZ1	1:E:245:ASN:HB3	1.55	0.72
2:I:15:SER:O	2:I:16:LYS:O	2.08	0.72
1:E:176:ILE:O	3:E:355:HOH:O	2.08	0.71
1:E:64:GLN:HE22	1:E:66:ARG:HH21	1.39	0.71
1:E:64:GLN:NE2	1:E:66:ARG:HH21	1.89	0.71
1:E:186:GLU:HG3	3:E:276:HOH:O	1.89	0.71
1:E:146:SER:HB3	1:E:220:CYS:O	1.90	0.71
2:I:17:PRO:O	2:I:20:ASP:CB	2.37	0.70
1:E:17:VAL:HG11	3:E:305:HOH:O	1.89	0.70
1:E:188(A):GLY:H	1:E:221(A):ALA:HB1	1.57	0.70
1:E:93:SER:HB2	1:E:101:ASN:ND2	2.06	0.70
1:E:132:ALA:HA	1:E:162:ILE:HG22	1.72	0.70
1:E:135:GLN:HG3	3:E:367:HOH:O	1.92	0.69
1:E:72:ASN:O	3:E:381:HOH:O	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:ASN:HB3	3:E:348:HOH:O	1.92	0.69
2:I:21:GLN:HB3	2:I:35:SER:OG	1.93	0.69
2:I:67:PHE:CD1	2:I:68:CYS:N	2.62	0.68
1:E:186:GLU:HB2	3:E:276:HOH:O	1.94	0.68
1:E:117:ARG:HD3	3:E:348:HOH:O	1.94	0.68
1:E:238:ILE:CG2	1:E:242:ILE:CD1	2.72	0.68
1:E:166:SER:O	1:E:170:SER:OG	2.12	0.67
1:E:138:ILE:HG12	1:E:199:VAL:HG22	1.76	0.67
1:E:99:LEU:HD12	1:E:215:TRP:CD1	2.30	0.67
1:E:215:TRP:CZ3	2:I:23:SER:OG	2.48	0.66
1:E:31:VAL:HG13	1:E:65:VAL:HG13	1.75	0.66
1:E:165:ASP:O	1:E:169:LYS:HB2	1.96	0.66
1:E:238:ILE:HG23	1:E:242:ILE:HD12	1.78	0.66
2:I:67:PHE:CZ	2:I:68:CYS:O	2.49	0.66
1:E:165:ASP:OD2	1:E:169:LYS:HD2	1.97	0.65
1:E:25:ASN:CG	1:E:25:ASN:O	2.33	0.64
2:I:19:CYS:CA	2:I:36:ASP:OD1	2.46	0.63
2:I:37:ILE:O	2:I:38:ARG:CG	2.46	0.63
1:E:48:ASN:ND2	1:E:50:GLN:H	1.97	0.62
2:I:18:CYS:O	2:I:69:TYR:CE2	2.50	0.62
1:E:25:ASN:ND2	1:E:25:ASN:O	2.33	0.62
1:E:51:TRP:CZ2	1:E:107:LYS:HD2	2.35	0.62
2:I:17:PRO:O	2:I:20:ASP:N	2.32	0.61
1:E:243:ALA:HB2	3:E:266:HOH:O	2.00	0.61
2:I:67:PHE:CG	2:I:68:CYS:N	2.50	0.61
1:E:64:GLN:HE21	1:E:66:ARG:HE	1.48	0.60
1:E:238:ILE:O	1:E:242:ILE:HD12	2.01	0.60
2:I:13:GLU:HG3	2:I:14:SER:CB	2.32	0.60
1:E:25:ASN:HB2	1:E:117:ARG:HB3	1.83	0.60
1:E:39:TYR:CE2	1:E:41:PHE:HB3	2.37	0.60
1:E:163:LEU:HD12	1:E:182:CYS:CB	2.31	0.60
1:E:17:VAL:HG22	1:E:144:THR:C	2.22	0.60
1:E:17:VAL:O	1:E:188:LYS:HA	2.02	0.60
1:E:99:LEU:CD1	1:E:215:TRP:CD1	2.85	0.59
1:E:195:SER:OG	2:I:26:LYS:C	2.40	0.59
1:E:31:VAL:HG22	1:E:67:LEU:CD2	2.32	0.59
1:E:138:ILE:CG1	1:E:199:VAL:HG22	2.33	0.59
1:E:87:LYS:NZ	1:E:245:ASN:HB3	2.17	0.59
1:E:192:GLN:CG	3:E:247:HOH:O	2.45	0.59
1:E:24:ALA:O	1:E:26:THR:HG23	2.03	0.58
1:E:20:TYR:HA	3:E:254:HOH:O	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:56:ALA:HB1	1:E:90:VAL:HG13	1.84	0.58
1:E:238:ILE:CG2	1:E:242:ILE:HD12	2.31	0.58
1:E:31:VAL:HG11	1:E:65:VAL:HG13	1.84	0.58
2:I:22:CYS:SG	2:I:22:CYS:O	2.62	0.57
1:E:101:ASN:HA	1:E:234:TYR:OH	2.05	0.57
1:E:163:LEU:HD12	1:E:182:CYS:HB2	1.86	0.57
1:E:145:LYS:HB2	1:E:147:SER:O	2.05	0.56
1:E:95:ASN:O	1:E:99:LEU:N	2.38	0.56
1:E:48:ASN:C	1:E:48:ASN:HD22	2.08	0.56
1:E:186:GLU:CB	3:E:276:HOH:O	2.53	0.56
1:E:70:GLU:HB2	3:E:261:HOH:O	2.06	0.56
1:E:25:ASN:N	3:E:316:HOH:O	2.39	0.55
1:E:80:GLU:HB3	1:E:82:PHE:HE2	1.66	0.55
1:E:235:VAL:O	1:E:239:LYS:HG3	2.06	0.55
1:E:99:LEU:HD12	1:E:215:TRP:CG	2.41	0.55
1:E:136:CYS:HB3	1:E:200:VAL:O	2.07	0.55
1:E:158:LEU:HD21	1:E:188:LYS:HB3	1.86	0.55
2:I:33:ARG:NH1	2:I:33:ARG:HG3	2.08	0.55
1:E:221:GLN:O	1:E:224:LYS:HB2	2.07	0.55
1:E:191:CYS:O	2:I:26:LYS:HB3	2.07	0.55
1:E:135:GLN:HE22	1:E:159:LYS:HD3	1.73	0.54
2:I:16:LYS:O	2:I:20:ASP:HB2	2.08	0.54
2:I:19:CYS:N	2:I:36:ASP:OD1	2.40	0.54
1:E:47:ILE:HG22	1:E:121:ILE:HG22	1.91	0.53
2:I:21:GLN:O	2:I:34:CYS:CA	2.53	0.53
1:E:135:GLN:HE22	1:E:159:LYS:CD	2.22	0.53
1:E:32:SER:HB3	1:E:66:ARG:HB2	1.91	0.53
1:E:64:GLN:HE22	1:E:66:ARG:NH2	2.05	0.53
1:E:149:THR:HG23	1:E:151:TYR:CD2	2.41	0.53
1:E:164:SER:CB	1:E:166:SER:OG	2.51	0.52
1:E:162:ILE:HD13	1:E:181:PHE:CE1	2.45	0.52
1:E:100:ASN:ND2	1:E:179:ASN:HB2	2.23	0.52
1:E:47:ILE:HG22	1:E:121:ILE:CG2	2.40	0.52
1:E:28:PRO:HB2	1:E:119:ALA:H	1.75	0.52
1:E:162:ILE:CD1	1:E:181:PHE:CE1	2.93	0.52
1:E:186:GLU:CG	3:E:276:HOH:O	2.53	0.51
1:E:29:TYR:HB3	1:E:119:ALA:O	2.11	0.51
1:E:78:GLY:N	1:E:80:GLU:OE1	2.32	0.51
1:E:21:THR:OG1	1:E:156:LYS:HE2	2.10	0.51
1:E:23:GLY:O	1:E:26:THR:HG23	2.10	0.51
1:E:240:GLN:NE2	3:E:298:HOH:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:THR:CG2	1:E:151:TYR:CE2	2.81	0.51
1:E:188(A):GLY:N	1:E:221(A):ALA:HB1	2.25	0.51
1:E:79:ASN:CG	1:E:117:ARG:HD2	2.31	0.51
1:E:163:LEU:HD12	1:E:182:CYS:HB3	1.93	0.50
1:E:134:THR:O	1:E:161:PRO:HA	2.12	0.50
1:E:165:ASP:OD1	1:E:169:LYS:HE3	2.11	0.50
2:I:28:MET:HA	2:I:28:MET:CE	2.37	0.49
2:I:21:GLN:HB3	2:I:35:SER:CB	2.41	0.49
1:E:28:PRO:HB3	1:E:117:ARG:O	2.12	0.49
1:E:64:GLN:NE2	1:E:66:ARG:NH2	2.60	0.49
1:E:114:LEU:HA	1:E:118:VAL:O	2.13	0.49
1:E:59:TYR:C	1:E:59:TYR:CD2	2.85	0.49
2:I:13:GLU:HG2	2:I:14:SER:N	2.24	0.49
1:E:95:ASN:ND2	3:E:287:HOH:O	2.45	0.49
1:E:221(A):ALA:HA	3:E:302:HOH:O	2.13	0.48
1:E:211:GLY:HA2	1:E:229:THR:O	2.14	0.48
1:E:81:GLN:OE1	1:E:112:ALA:HB1	2.14	0.48
1:E:45:SER:O	1:E:52:VAL:HA	2.14	0.48
1:E:80:GLU:CB	1:E:82:PHE:CE2	2.95	0.48
1:E:144:THR:OG1	1:E:145:LYS:HD3	2.14	0.48
2:I:18:CYS:HB3	2:I:71:PRO:HG2	1.96	0.47
1:E:223:ASN:O	1:E:224:LYS:HD2	2.13	0.47
1:E:64:GLN:NE2	1:E:66:ARG:HE	2.12	0.47
2:I:67:PHE:CE1	2:I:68:CYS:O	2.67	0.47
2:I:28:MET:HE1	2:I:29:PRO:CA	2.41	0.47
1:E:87:LYS:HZ1	1:E:245:ASN:CB	2.25	0.47
2:I:16:LYS:H	2:I:16:LYS:HG2	1.49	0.47
1:E:25:ASN:HB2	1:E:117:ARG:CB	2.44	0.47
1:E:100:ASN:ND2	1:E:177:THR:OG1	2.48	0.47
2:I:28:MET:HE2	2:I:30:PRO:HD3	1.97	0.46
1:E:56:ALA:HB1	1:E:90:VAL:CG1	2.45	0.46
1:E:83:ILE:CG2	1:E:110:SER:HB2	2.41	0.46
2:I:13:GLU:HG3	2:I:14:SER:CA	2.45	0.46
1:E:141:TRP:CD2	1:E:155:LEU:HD23	2.51	0.46
2:I:19:CYS:H	2:I:36:ASP:CG	2.19	0.46
1:E:82:PHE:N	1:E:82:PHE:CD2	2.81	0.46
1:E:163:LEU:HD21	1:E:184(A):GLY:O	2.15	0.46
1:E:123:LEU:HD12	1:E:123:LEU:HA	1.82	0.46
2:I:67:PHE:HZ	2:I:70:GLU:HB2	1.81	0.46
1:E:22:CYS:HB3	1:E:26:THR:OG1	2.16	0.46
2:I:16:LYS:HB3	2:I:17:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:ASN:CB	3:E:348:HOH:O	2.58	0.45
1:E:99:LEU:CD1	1:E:215:TRP:CG	2.99	0.45
1:E:48:ASN:HD21	1:E:50:GLN:H	1.64	0.45
1:E:219:GLY:CA	3:E:303:HOH:O	2.65	0.45
1:E:133:GLY:N	1:E:162:ILE:O	2.40	0.45
1:E:87:LYS:HB3	1:E:107:LYS:HB3	1.99	0.45
1:E:203:GLY:N	3:E:338:HOH:O	2.50	0.45
1:E:98:THR:C	1:E:100:ASN:H	2.21	0.44
2:I:27:SER:OG	2:I:30:PRO:HA	2.17	0.44
1:E:236:SER:O	1:E:240:GLN:HB2	2.18	0.44
1:E:213:VAL:HA	1:E:228:TYR:CD1	2.52	0.44
1:E:71:ASP:HB3	1:E:77:GLU:OE1	2.18	0.44
1:E:179:ASN:OD1	1:E:233:ASN:ND2	2.43	0.44
1:E:16:ILE:HD11	1:E:138:ILE:HG22	1.99	0.44
2:I:29:PRO:HB2	2:I:65:ASN:N	2.33	0.44
2:I:13:GLU:HG3	2:I:14:SER:HB3	2.00	0.44
1:E:16:ILE:CD1	1:E:138:ILE:HG22	2.48	0.44
1:E:189:ASP:OD2	1:E:190:SER:N	2.51	0.44
2:I:21:GLN:O	2:I:34:CYS:SG	2.76	0.44
2:I:70:GLU:HA	2:I:71:PRO:HA	1.95	0.43
1:E:230:LYS:NZ	3:E:366:HOH:O	2.48	0.43
2:I:37:ILE:C	2:I:38:ARG:CG	2.86	0.43
2:I:73:LYS:HD3	2:I:73:LYS:HA	1.70	0.43
1:E:34:ASN:HB2	3:E:269:HOH:O	2.18	0.43
2:I:17:PRO:O	2:I:20:ASP:CA	2.66	0.43
2:I:28:MET:CE	2:I:30:PRO:HD3	2.49	0.43
1:E:221:GLN:HB3	1:E:224:LYS:CB	2.49	0.43
1:E:238:ILE:O	1:E:242:ILE:HB	2.19	0.42
1:E:224:LYS:N	1:E:224:LYS:CD	2.70	0.42
1:E:83:ILE:HD11	3:E:304:HOH:O	2.20	0.42
2:I:16:LYS:O	2:I:20:ASP:CB	2.66	0.42
1:E:138:ILE:O	1:E:139:SER:HB3	2.19	0.42
1:E:41:PHE:CE2	1:E:60:LYS:HD2	2.54	0.42
1:E:17:VAL:HG12	1:E:188(A):GLY:O	2.20	0.42
1:E:116:SER:OG	1:E:117:ARG:N	2.52	0.42
2:I:72:CYS:SG	2:I:73:LYS:C	2.98	0.42
1:E:48:ASN:HD22	1:E:49:SER:H	1.61	0.41
1:E:105:LEU:HD22	1:E:237:TRP:CZ3	2.54	0.41
1:E:121:ILE:CG2	1:E:209:LEU:HD22	2.46	0.41
1:E:145:LYS:C	1:E:147:SER:N	2.73	0.41
1:E:188:LYS:O	1:E:189:ASP:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:GLN:NE2	1:E:159:LYS:HD3	2.33	0.41
1:E:16:ILE:HG21	1:E:158:LEU:HB2	2.03	0.41
1:E:29:TYR:O	1:E:31:VAL:HG23	2.21	0.41
1:E:82:PHE:C	1:E:83:ILE:HG12	2.40	0.41
2:I:65:ASN:OD1	2:I:66:ASP:OD2	2.39	0.41
1:E:201:CYS:SG	1:E:210:GLN:HG3	2.61	0.40
1:E:37:SER:OG	1:E:60:LYS:HE2	2.20	0.40
1:E:135:GLN:NE2	1:E:159:LYS:CD	2.83	0.40
2:I:29:PRO:HA	2:I:30:PRO:HD3	1.96	0.40
1:E:57:HIS:CD2	2:I:27:SER:HB3	2.56	0.40
1:E:48:ASN:C	1:E:48:ASN:ND2	2.73	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:170:SER:CB	3:E:295:HOH:O[3_645]	0.55	1.65
1:E:170:SER:CA	3:E:295:HOH:O[3_645]	1.78	0.42
1:E:170:SER:OG	3:E:295:HOH:O[3_645]	1.96	0.24
3:E:297:HOH:O	3:E:300:HOH:O[6_555]	2.12	0.08
1:E:74:ASN:ND2	1:E:90:VAL:CG2[6_455]	2.18	0.02

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	E	221/223 (99%)	202 (91%)	19 (9%)	0	100 100
2	I	32/82 (39%)	13 (41%)	7 (22%)	12 (38%)	0 0
All	All	253/305 (83%)	215 (85%)	26 (10%)	12 (5%)	3 1

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	16	LYS
2	I	17	PRO
2	I	18	CYS
2	I	37	ILE
2	I	66	ASP
2	I	67	PHE
2	I	68	CYS
2	I	70	GLU
2	I	71	PRO
2	I	72	CYS
2	I	21	GLN
2	I	36	ASP

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	E	184/184 (100%)	154 (84%)	30 (16%)	3 3
2	I	36/78 (46%)	27 (75%)	9 (25%)	1 0
All	All	220/262 (84%)	181 (82%)	39 (18%)	2 2

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	25	ASN
1	E	45	SER
1	E	48	ASN
1	E	49	SER
1	E	59	TYR
1	E	74	ASN
1	E	83	ILE
1	E	101	ASN
1	E	116	SER
1	E	117	ARG
1	E	121	ILE
1	E	123	LEU

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Mol	Chain	Res	Type
1	E	135	GLN
1	E	145	LYS
1	E	146	SER
1	E	154	VAL
1	E	155	LEU
1	E	158	LEU
1	E	164	SER
1	E	165	ASP
1	E	170	SER
1	E	177	THR
1	E	192	GLN
1	E	200	VAL
1	E	201	CYS
1	E	202	SER
1	E	210	GLN
1	E	221	GLN
1	E	224	LYS
1	E	244	SER
2	I	20	ASP
2	I	21	GLN
2	I	28	MET
2	I	33	ARG
2	I	66	ASP
2	I	67	PHE
2	I	71	PRO
2	I	72	CYS
2	I	73	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	30	GLN
1	E	48	ASN
1	E	64	GLN
1	E	100	ASN
1	E	135	GLN
1	E	192	GLN
1	E	240	GLN
2	I	65	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.