Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:51 AM GMT

PDB ID	:	2OHC
Title	:	structural and mutational analysis of tRNA-intron splicing endonuclease from Thermoplasma acidophilum DSM1728
Authors	:	Kim, Y.K.; Mizutani, K.; Rhee, K.H.; Lee, W.H.; Park, S.Y.; Hwang, K.Y.
Deposited on	:	2007-01-10
Resolution	:	2.50 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:

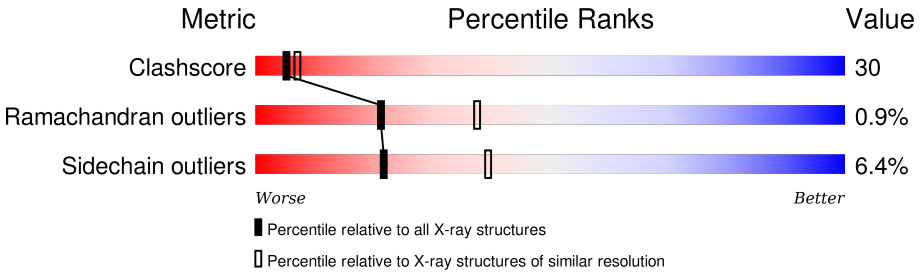
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.50 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	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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	289	54% 40% 6%
1	B	289	55% 39% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4998 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 tRNA-splicing endonuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2347	1504	396	438	9			
1	B	288	Total	C	N	O	S	0	0	0
			2339	1499	395	437	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	146	GLY	ALA	CONFLICT	UNP Q9HIY5
B	146	GLY	ALA	CONFLICT	UNP Q9HIY5

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	162	Total	O	0	0
			162	162		
2	B	150	Total	O	0	0
			150	150		

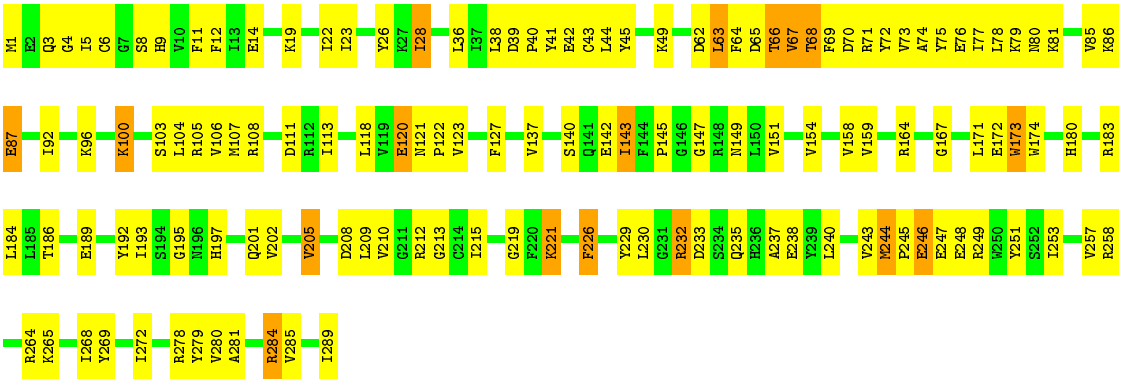
3 Residue-property plots (i)

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.

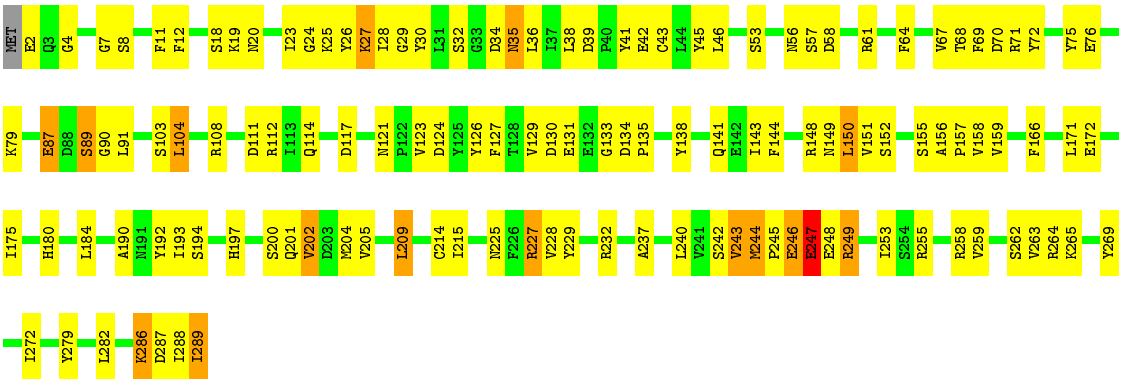
- Molecule 1: tRNA-splicing endonuclease

Chain A:



- Molecule 1: tRNA-splicing endonuclease

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 21 2	Depositor
Cell constants a, b, c, α, β, γ	57.17Å 57.17Å 459.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.50	Depositor
% Data completeness (in resolution range)	90.9 (19.99-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.224 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4998	wwPDB-VP
Average B, all atoms (Å^2)	44.0	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	0.38	0/2403	0.63	2/3240 (0.1%)
1	B	0.48	2/2395 (0.1%)	0.66	3/3230 (0.1%)
All	All	0.43	2/4798 (0.0%)	0.65	5/6470 (0.1%)

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	0	2
1	B	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	243	VAL	CB-CG2	-6.54	1.39	1.52
1	B	243	VAL	CB-CG1	-5.68	1.41	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	247	GLU	N-CA-C	-9.83	84.45	111.00
1	B	244	MET	CG-SD-CE	-6.70	89.48	100.20
1	A	143	ILE	N-CA-C	5.50	125.85	111.00
1	A	65	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	227	ARG	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	66	THR	Peptide
1	A	72	TYR	Sidechain
1	B	246	GLU	Peptide
1	B	247	GLU	Peptide

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	2347	0	2288	130	0
1	B	2339	0	2276	155	1
2	A	162	0	0	7	0
2	B	150	0	0	4	0
All	All	4998	0	4564	280	1

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 30.

All (280) 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:246:GLU:CB	1:B:247:GLU:HG3	1.46	1.46
1:B:246:GLU:HB3	1:B:247:GLU:CG	1.60	1.30
1:A:62:ASP:O	1:A:66:THR:HG23	1.38	1.18
1:A:64:PHE:O	1:A:67:VAL:O	1.59	1.18
1:B:246:GLU:HB3	1:B:247:GLU:CB	1.75	1.16
1:B:246:GLU:CG	1:B:247:GLU:HG3	1.80	1.12
1:B:27:LYS:HA	1:B:27:LYS:HE3	1.22	1.09
1:B:246:GLU:HB3	1:B:247:GLU:HG3	1.09	1.05
1:B:215:ILE:HG13	1:B:229:TYR:HB2	1.38	1.01
1:B:56:ASN:HD22	1:B:58:ASP:H	1.08	1.01
1:B:246:GLU:CB	1:B:247:GLU:CG	2.29	0.98
1:B:215:ILE:CG1	1:B:229:TYR:HB2	1.94	0.96
1:A:44:LEU:HD21	1:A:63:LEU:HB3	1.48	0.94
1:B:150:LEU:H	1:B:150:LEU:HD23	1.30	0.94
1:B:29:GLY:HA3	1:B:38:LEU:HD12	1.52	0.91
1:B:246:GLU:CG	1:B:247:GLU:CG	2.49	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ILE:HD13	1:A:268:ILE:HD12	1.57	0.85
1:A:63:LEU:O	1:A:67:VAL:HG12	1.78	0.83
1:B:23:ILE:HD11	1:B:36:LEU:HD11	1.61	0.81
1:A:62:ASP:O	1:A:66:THR:CG2	2.25	0.81
1:B:246:GLU:HG2	1:B:247:GLU:HG3	1.63	0.80
1:B:264:ARG:HG2	1:B:264:ARG:O	1.80	0.80
1:B:87:GLU:CD	1:B:87:GLU:H	1.86	0.78
1:A:253:ILE:O	1:A:257:VAL:HG23	1.84	0.77
1:B:150:LEU:CD2	1:B:150:LEU:H	1.97	0.77
1:A:249:ARG:HD2	1:A:249:ARG:N	1.99	0.75
1:A:120:GLU:O	1:A:122:PRO:HD3	1.87	0.74
1:B:288:ILE:HG12	1:B:289:ILE:HG23	1.70	0.74
1:A:215:ILE:HB	1:A:229:TYR:HB2	1.70	0.74
1:A:81:LYS:HE3	1:A:289:ILE:HB	1.69	0.73
1:A:205:VAL:O	1:A:209:LEU:HD23	1.90	0.72
1:A:201:GLN:O	1:A:205:VAL:HG12	1.88	0.71
1:B:41:TYR:CG	1:B:87:GLU:HG2	2.25	0.71
2:A:362:HOH:O	1:B:255:ARG:HD3	1.91	0.71
1:B:56:ASN:ND2	1:B:58:ASP:H	1.84	0.71
1:B:71:ARG:HD2	1:B:90:GLY:HA2	1.73	0.69
1:B:286:LYS:HE2	1:B:286:LYS:H	1.57	0.69
1:B:23:ILE:HD11	1:B:36:LEU:CD1	2.22	0.69
1:B:19:LYS:HE3	1:B:34:ASP:C	2.13	0.69
1:A:87:GLU:H	1:A:87:GLU:CD	1.95	0.69
1:B:286:LYS:HE2	1:B:287:ASP:N	2.08	0.69
1:A:158:VAL:HG22	1:A:193:ILE:HD11	1.74	0.69
1:A:257:VAL:HG12	1:A:284:ARG:HD2	1.75	0.68
1:B:264:ARG:HH21	1:B:265:LYS:NZ	1.92	0.68
1:B:263:VAL:O	1:B:264:ARG:HB3	1.93	0.68
1:A:186:THR:OG1	1:A:189:GLU:HG3	1.93	0.68
1:B:246:GLU:HG2	1:B:247:GLU:CG	2.23	0.67
1:A:240:LEU:HD13	1:A:265:LYS:HD2	1.77	0.67
1:B:246:GLU:HB3	1:B:247:GLU:CA	2.24	0.67
1:A:113:ILE:HG21	1:A:253:ILE:HD12	1.77	0.67
1:B:56:ASN:ND2	1:B:57:SER:H	1.92	0.67
1:B:264:ARG:HH21	1:B:265:LYS:HZ3	1.42	0.67
1:B:28:ILE:HD12	1:B:42:GLU:HB3	1.77	0.66
1:A:205:VAL:HG11	1:A:243:VAL:HG22	1.76	0.66
1:B:19:LYS:O	1:B:23:ILE:HD13	1.96	0.66
1:A:258:ARG:NH1	1:A:284:ARG:HH12	1.93	0.66
1:B:32:SER:HA	2:B:393:HOH:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:GLU:HB3	1:B:247:GLU:HB2	1.75	0.66
1:A:41:TYR:CE2	1:A:87:GLU:HG2	2.31	0.65
1:B:263:VAL:HG23	1:B:265:LYS:HG3	1.79	0.64
1:B:29:GLY:HA3	1:B:38:LEU:CD1	2.25	0.64
1:A:71:ARG:HG2	1:A:106:VAL:HG21	1.79	0.64
1:A:143:ILE:HG12	1:A:279:TYR:HB2	1.80	0.64
1:A:73:VAL:O	1:A:77:ILE:HD13	1.98	0.64
1:B:225:ASN:HD22	1:B:242:SER:HA	1.62	0.64
1:B:103:SER:HB2	1:B:124:ASP:H	1.61	0.64
1:B:172:GLU:O	1:B:175:ILE:HG22	1.97	0.63
1:B:246:GLU:HB2	1:B:247:GLU:HG3	1.69	0.63
1:B:150:LEU:HD23	1:B:150:LEU:N	2.09	0.63
1:A:137:VAL:HG13	1:A:285:VAL:HB	1.80	0.62
1:A:219:GLY:N	1:A:226:PHE:HA	2.15	0.62
1:B:112:ARG:NH1	1:B:249:ARG:HE	1.97	0.62
1:B:112:ARG:HH22	1:B:249:ARG:HH21	1.46	0.61
1:A:39:ASP:OD2	1:A:42:GLU:HG3	2.00	0.61
1:B:26:TYR:O	1:B:28:ILE:HG23	1.99	0.61
1:B:45:TYR:HA	1:B:72:TYR:OH	2.01	0.60
1:B:215:ILE:CD1	1:B:229:TYR:HB2	2.31	0.60
1:B:159:VAL:HG13	1:B:166:PHE:HB2	1.83	0.60
1:B:157:PRO:HD2	2:B:302:HOH:O	2.02	0.60
1:A:121:ASN:C	1:A:123:VAL:H	2.04	0.60
1:A:171:LEU:HB2	1:A:183:ARG:NH1	2.17	0.60
1:A:149:ASN:ND2	1:A:215:ILE:HG12	2.16	0.59
1:B:19:LYS:HE3	1:B:35:ASN:N	2.16	0.59
1:B:288:ILE:HG12	1:B:289:ILE:CG2	2.32	0.59
1:B:25:LYS:HE2	2:B:438:HOH:O	2.02	0.59
1:B:249:ARG:HG2	1:B:249:ARG:HH11	1.67	0.59
1:B:27:LYS:CA	1:B:27:LYS:HE3	2.09	0.59
1:B:108:ARG:HB3	1:B:111:ASP:OD2	2.02	0.58
1:A:232:ARG:HD2	1:A:233:ASP:N	2.18	0.58
1:A:22:ILE:HG21	1:A:36:LEU:HD21	1.85	0.58
1:A:105:ARG:CZ	1:A:107:MET:SD	2.91	0.58
1:B:68:THR:HG22	1:B:69:PHE:H	1.69	0.58
1:B:112:ARG:HH12	1:B:249:ARG:NH2	2.02	0.58
1:A:208:ASP:O	1:A:212:ARG:HG2	2.04	0.58
1:B:158:VAL:HG22	1:B:193:ILE:HD11	1.86	0.57
1:A:192:TYR:O	1:A:197:HIS:HE1	1.87	0.57
1:A:44:LEU:CD2	1:A:63:LEU:HB3	2.30	0.57
1:B:204:MET:HE2	1:B:204:MET:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:LYS:H	1:B:286:LYS:CE	2.18	0.57
1:A:221:LYS:HD2	1:A:221:LYS:H	1.68	0.57
1:B:244:MET:SD	1:B:248:GLU:HG2	2.44	0.57
1:B:23:ILE:O	1:B:27:LYS:HA	2.05	0.57
1:B:149:ASN:OD1	1:B:232:ARG:HA	2.05	0.57
1:A:22:ILE:HG22	1:A:23:ILE:N	2.20	0.57
1:B:4:GLY:N	1:B:35:ASN:HD21	2.02	0.56
1:B:112:ARG:NH2	1:B:249:ARG:HH21	2.02	0.56
1:B:192:TYR:O	1:B:197:HIS:HE1	1.87	0.56
1:B:64:PHE:O	1:B:67:VAL:O	2.23	0.56
1:A:66:THR:HG22	2:A:415:HOH:O	2.05	0.56
1:A:205:VAL:HG11	1:A:243:VAL:CG2	2.36	0.56
1:B:89:SER:C	1:B:91:LEU:H	2.09	0.55
1:A:103:SER:OG	1:A:123:VAL:HA	2.06	0.55
1:B:253:ILE:HG21	1:B:282:LEU:HD22	1.89	0.55
1:A:244:MET:HG2	1:A:248:GLU:OE2	2.07	0.55
1:B:143:ILE:HG12	1:B:144:PHE:N	2.22	0.55
1:B:190:ALA:O	1:B:194:SER:HB2	2.07	0.54
1:B:2:GLU:OE1	1:B:18:SER:HA	2.07	0.54
1:A:45:TYR:O	1:A:49:LYS:HG2	2.06	0.54
1:B:117:ASP:O	1:B:121:ASN:HB2	2.08	0.54
1:B:214:CYS:HB3	1:B:228:VAL:CG1	2.38	0.54
1:B:246:GLU:CG	1:B:247:GLU:HG2	2.36	0.54
1:A:118:LEU:HB3	1:A:280:VAL:HG11	1.89	0.54
1:A:147:GLY:HA3	1:A:213:GLY:O	2.08	0.54
1:B:130:ASP:OD1	1:B:134:ASP:HB2	2.08	0.53
1:A:230:LEU:HD12	1:A:238:GLU:HG3	1.89	0.53
1:A:164:ARG:NH1	1:B:131:GLU:HA	2.23	0.53
1:B:240:LEU:HD13	1:B:265:LYS:HD2	1.90	0.53
1:A:104:LEU:HD13	1:A:105:ARG:N	2.24	0.53
1:B:68:THR:HG22	1:B:69:PHE:N	2.23	0.53
1:A:147:GLY:HA3	1:A:213:GLY:C	2.28	0.53
1:B:28:ILE:HD11	1:B:46:LEU:HD11	1.90	0.53
1:B:286:LYS:HE2	1:B:287:ASP:H	1.73	0.53
1:B:70:ASP:HA	1:B:129:VAL:HG11	1.90	0.52
1:B:4:GLY:N	1:B:35:ASN:ND2	2.57	0.52
1:A:79:LYS:C	1:A:81:LYS:H	2.11	0.52
1:B:225:ASN:ND2	1:B:243:VAL:H	2.08	0.52
1:B:2:GLU:O	1:B:12:PHE:HA	2.10	0.52
1:B:286:LYS:HE2	1:B:286:LYS:N	2.22	0.52
1:A:240:LEU:HD13	1:A:265:LYS:CD	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:ILE:O	1:B:27:LYS:HE3	2.10	0.51
1:A:105:ARG:NE	1:A:107:MET:SD	2.84	0.51
1:A:221:LYS:HD2	1:A:221:LYS:N	2.26	0.51
1:B:56:ASN:HD22	1:B:58:ASP:N	1.92	0.50
1:B:249:ARG:CG	1:B:249:ARG:HH11	2.23	0.50
1:A:105:ARG:HA	2:A:292:HOH:O	2.12	0.50
1:B:104:LEU:HD11	1:B:127:PHE:HB2	1.93	0.50
1:B:197:HIS:O	1:B:204:MET:HE2	2.11	0.50
1:B:30:TYR:O	1:B:36:LEU:HD12	2.12	0.50
1:B:24:GLY:HA2	1:B:27:LYS:HZ1	1.76	0.50
1:B:75:TYR:CD2	1:B:87:GLU:HG3	2.46	0.50
1:A:68:THR:HG22	1:A:71:ARG:H	1.76	0.50
1:A:232:ARG:HD2	1:A:233:ASP:H	1.75	0.50
1:A:247:GLU:HB2	2:A:294:HOH:O	2.10	0.50
1:B:258:ARG:HG2	1:B:258:ARG:HH11	1.77	0.50
1:A:40:PRO:HB3	1:A:63:LEU:HD12	1.94	0.49
1:B:7:GLY:O	1:B:8:SER:HB2	2.12	0.49
1:B:259:VAL:O	1:B:262:SER:HB3	2.13	0.49
1:B:23:ILE:HG22	1:B:27:LYS:NZ	2.28	0.49
1:B:19:LYS:HD2	1:B:36:LEU:N	2.28	0.49
1:A:249:ARG:HD2	1:A:249:ARG:H	1.77	0.49
1:B:112:ARG:NH1	1:B:249:ARG:NE	2.61	0.48
1:A:64:PHE:HA	1:A:67:VAL:HG12	1.94	0.48
1:A:66:THR:HG21	2:A:417:HOH:O	2.13	0.48
1:A:5:ILE:HA	1:A:9:HIS:O	2.13	0.48
1:B:156:ALA:HB1	1:B:157:PRO:HD2	1.94	0.48
1:B:201:GLN:HG3	1:B:272:ILE:HG13	1.94	0.48
1:A:74:ALA:O	1:A:78:LEU:HG	2.13	0.48
1:A:39:ASP:C	1:A:39:ASP:OD2	2.51	0.48
1:A:69:PHE:CZ	1:B:184:LEU:HD22	2.48	0.48
1:B:112:ARG:HH12	1:B:249:ARG:HH21	1.61	0.48
1:A:245:PRO:O	1:A:247:GLU:N	2.47	0.48
1:B:245:PRO:HG2	1:B:248:GLU:OE1	2.14	0.48
1:A:121:ASN:C	1:A:123:VAL:N	2.67	0.47
1:A:76:GLU:OE2	1:B:180:HIS:NE2	2.40	0.47
1:A:202:VAL:HA	1:A:243:VAL:HG21	1.96	0.47
1:A:195:GLY:HA2	1:A:197:HIS:CE1	2.49	0.47
1:B:38:LEU:HD21	1:B:46:LEU:HD12	1.97	0.47
1:A:164:ARG:HD2	1:A:184:LEU:HD11	1.96	0.47
1:A:108:ARG:O	1:A:111:ASP:HB2	2.14	0.47
1:B:2:GLU:OE2	1:B:19:LYS:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ILE:HG13	1:A:145:PRO:HD3	1.95	0.47
1:A:289:ILE:N	2:A:364:HOH:O	2.39	0.47
1:B:112:ARG:NH1	1:B:249:ARG:HH21	2.13	0.47
1:A:142:GLU:HG3	1:A:279:TYR:O	2.15	0.46
1:A:100:LYS:HE3	1:A:100:LYS:HA	1.96	0.46
1:A:85:VAL:CG1	1:A:92:ILE:HG23	2.46	0.46
1:A:6:CYS:O	1:A:8:SER:N	2.48	0.46
1:B:215:ILE:HD11	1:B:229:TYR:CB	2.46	0.46
1:B:264:ARG:CG	1:B:264:ARG:O	2.57	0.46
1:B:172:GLU:HB2	1:B:175:ILE:HG22	1.98	0.46
1:A:221:LYS:CD	1:A:221:LYS:H	2.27	0.46
1:A:154:VAL:HG23	1:A:154:VAL:O	2.14	0.46
1:A:151:VAL:HG13	1:A:213:GLY:HA2	1.97	0.46
1:A:237:ALA:O	1:A:265:LYS:NZ	2.36	0.46
1:B:152:SER:HB2	1:B:172:GLU:OE1	2.15	0.46
1:A:180:HIS:NE2	1:B:76:GLU:OE2	2.47	0.46
1:A:172:GLU:HG2	1:A:174:TRP:NE1	2.31	0.46
1:B:23:ILE:HG22	1:B:27:LYS:HZ3	1.80	0.45
1:A:19:LYS:O	1:A:23:ILE:HG13	2.15	0.45
1:A:41:TYR:CD2	1:A:87:GLU:HG2	2.51	0.45
1:B:215:ILE:HD11	1:B:229:TYR:HB2	1.98	0.45
1:A:253:ILE:HA	1:A:269:TYR:OH	2.16	0.45
1:B:130:ASP:CG	1:B:134:ASP:HB2	2.36	0.45
1:A:85:VAL:HG13	1:A:92:ILE:HG23	1.98	0.45
1:B:112:ARG:HH12	1:B:249:ARG:CZ	2.29	0.45
1:A:96:LYS:HE3	1:A:96:LYS:HA	1.99	0.45
1:A:257:VAL:CG1	1:A:284:ARG:HD2	2.47	0.44
1:B:89:SER:C	1:B:91:LEU:N	2.71	0.44
1:A:75:TYR:CE2	1:A:85:VAL:HB	2.52	0.44
1:B:288:ILE:O	1:B:289:ILE:HG12	2.17	0.44
1:A:264:ARG:HG3	1:A:264:ARG:O	2.18	0.44
1:A:87:GLU:CD	1:A:87:GLU:N	2.68	0.44
1:A:40:PRO:O	1:A:44:LEU:HD23	2.18	0.44
1:A:173:TRP:CZ3	1:A:174:TRP:HB3	2.52	0.44
1:A:143:ILE:HG21	1:A:281:ALA:HB2	1.99	0.44
1:A:3:GLN:HB3	1:A:12:PHE:CD1	2.53	0.44
1:B:29:GLY:CA	1:B:38:LEU:HD12	2.36	0.44
1:B:155:SER:HA	1:B:193:ILE:O	2.18	0.44
1:B:11:PHE:HA	1:B:53:SER:O	2.17	0.44
1:A:209:LEU:HD22	1:A:279:TYR:OH	2.17	0.44
1:B:114:GLN:HB3	1:B:117:ASP:OD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:LEU:O	1:B:172:GLU:C	2.57	0.43
1:A:4:GLY:HA3	1:A:36:LEU:O	2.19	0.43
1:B:200:SER:OG	1:B:202:VAL:HG13	2.18	0.43
1:B:288:ILE:C	1:B:289:ILE:HG23	2.39	0.43
1:B:104:LEU:HD11	1:B:127:PHE:CB	2.48	0.43
1:B:258:ARG:HG2	1:B:258:ARG:NH1	2.34	0.43
1:B:133:GLY:O	1:B:135:PRO:HD3	2.18	0.43
1:B:23:ILE:HD12	1:B:23:ILE:N	2.33	0.43
1:A:68:THR:CG2	1:A:70:ASP:H	2.31	0.43
1:B:253:ILE:CG2	1:B:282:LEU:HD22	2.48	0.43
1:A:244:MET:HA	1:A:245:PRO:HD3	1.83	0.43
1:A:230:LEU:CD1	1:A:238:GLU:HG3	2.48	0.43
1:A:205:VAL:O	1:A:209:LEU:CD2	2.62	0.43
1:A:201:GLN:HG3	1:A:272:ILE:HG12	2.00	0.43
1:B:249:ARG:CG	1:B:249:ARG:NH1	2.80	0.43
1:A:245:PRO:O	1:A:246:GLU:C	2.55	0.43
1:A:159:VAL:HG13	1:B:61:ARG:NH2	2.33	0.43
1:A:104:LEU:HD11	1:A:127:PHE:CB	2.49	0.42
1:B:214:CYS:HB3	1:B:228:VAL:HG13	1.99	0.42
1:B:159:VAL:CG1	1:B:166:PHE:HB2	2.50	0.42
1:A:26:TYR:HB2	1:A:28:ILE:CD1	2.49	0.42
1:A:66:THR:OG1	1:A:67:VAL:N	2.52	0.42
1:B:130:ASP:OD2	1:B:134:ASP:N	2.53	0.42
1:B:7:GLY:O	1:B:8:SER:CB	2.67	0.42
1:B:79:LYS:HA	1:B:79:LYS:HD3	1.85	0.42
1:A:67:VAL:CG1	1:A:67:VAL:O	2.66	0.42
1:B:39:ASP:OD1	1:B:42:GLU:HG3	2.19	0.42
1:B:35:ASN:HA	1:B:35:ASN:HD22	1.66	0.42
1:A:201:GLN:HG3	1:A:272:ILE:CG1	2.50	0.42
1:B:23:ILE:C	1:B:27:LYS:HZ1	2.23	0.41
1:B:151:VAL:HG22	2:B:358:HOH:O	2.20	0.41
1:A:143:ILE:HD13	1:A:268:ILE:CD1	2.39	0.41
1:A:249:ARG:HB2	1:A:251:TYR:CE1	2.55	0.41
1:A:151:VAL:HG11	1:A:210:VAL:O	2.20	0.41
1:A:1:MET:N	2:A:445:HOH:O	2.52	0.41
1:A:71:ARG:HA	1:A:106:VAL:HG11	2.02	0.41
1:A:68:THR:HG23	1:A:70:ASP:H	1.85	0.41
1:A:167:GLY:HA3	1:A:171:LEU:HD11	2.01	0.41
1:B:4:GLY:HA2	1:B:35:ASN:ND2	2.35	0.41
1:A:120:GLU:C	1:A:122:PRO:HD3	2.39	0.41
1:A:154:VAL:O	1:A:154:VAL:CG2	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:TYR:HB2	1:B:138:TYR:HB2	2.03	0.41
1:B:227:ARG:HG2	1:B:237:ALA:CB	2.50	0.41
1:A:249:ARG:CD	1:A:249:ARG:N	2.78	0.41
1:A:120:GLU:H	1:A:120:GLU:HG3	1.63	0.41
1:A:68:THR:HG22	1:A:70:ASP:N	2.36	0.41
1:A:4:GLY:HA3	1:A:11:PHE:CZ	2.56	0.41
1:B:209:LEU:HD13	1:B:279:TYR:OH	2.21	0.41
1:A:113:ILE:CG2	1:A:253:ILE:HD12	2.49	0.40
1:A:142:GLU:HA	1:A:279:TYR:O	2.21	0.40
1:A:38:LEU:HB3	1:A:42:GLU:HB2	2.04	0.40
1:B:129:VAL:O	1:B:129:VAL:HG13	2.21	0.40
1:A:86:LYS:HB3	1:A:86:LYS:HE3	1.93	0.40
1:B:112:ARG:CZ	1:B:249:ARG:HH21	2.34	0.40
1:B:24:GLY:CA	1:B:27:LYS:HZ1	2.34	0.40
1:B:39:ASP:OD1	1:B:39:ASP:C	2.59	0.40
1:B:245:PRO:CG	1:B:248:GLU:OE1	2.70	0.40
1:B:269:TYR:HD2	1:B:282:LEU:HD13	1.86	0.40
1:A:264:ARG:HD2	1:A:264:ARG:HA	1.90	0.40

All (1) 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:B:20:ASN:OD1	1:B:232:ARG:NH1[8_662]	1.79	0.41

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	287/289 (99%)	261 (91%)	22 (8%)	4 (1%)	14 24
1	B	286/289 (99%)	259 (91%)	26 (9%)	1 (0%)	46 68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	573/578 (99%)	520 (91%)	48 (8%)	5 (1%)	21 37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	173	TRP
1	A	246	GLU
1	B	89	SER
1	A	235	GLN

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	252/252 (100%)	235 (93%)	17 (7%)	20 37
1	B	251/252 (100%)	236 (94%)	15 (6%)	24 43
All	All	503/504 (100%)	471 (94%)	32 (6%)	22 39

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	28	ILE
1	A	43	CYS
1	A	63	LEU
1	A	67	VAL
1	A	68	THR
1	A	87	GLU
1	A	100	LYS
1	A	120	GLU
1	A	140	SER
1	A	205	VAL
1	A	221	LYS
1	A	226	PHE

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Mol	Chain	Res	Type
1	A	232	ARG
1	A	244	MET
1	A	278	ARG
1	A	284	ARG
1	B	27	LYS
1	B	35	ASN
1	B	43	CYS
1	B	87	GLU
1	B	104	LEU
1	B	123	VAL
1	B	141	GLN
1	B	148	ARG
1	B	150	LEU
1	B	202	VAL
1	B	205	VAL
1	B	209	LEU
1	B	249	ARG
1	B	286	LYS
1	B	289	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	GLN
1	A	197	HIS
1	B	3	GLN
1	B	35	ASN
1	B	56	ASN
1	B	114	GLN
1	B	188	ASN
1	B	197	HIS
1	B	225	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

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.