Full wwPDB X-ray Structure Validation Report ⓘ

Jan 11, 2024 – 12:08 PM JST

PDB ID	:	8JH1
Title	:	Crystal Structure of the Csm6 Y161A mutant from Thermus thermophilus HB8 in complex with cyclic-tetraadenylate (cA4)
Authors	:	Lin, Z.; Du, L.
Deposited on	:	2023-05-22
Resolution	:	2.89 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
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:

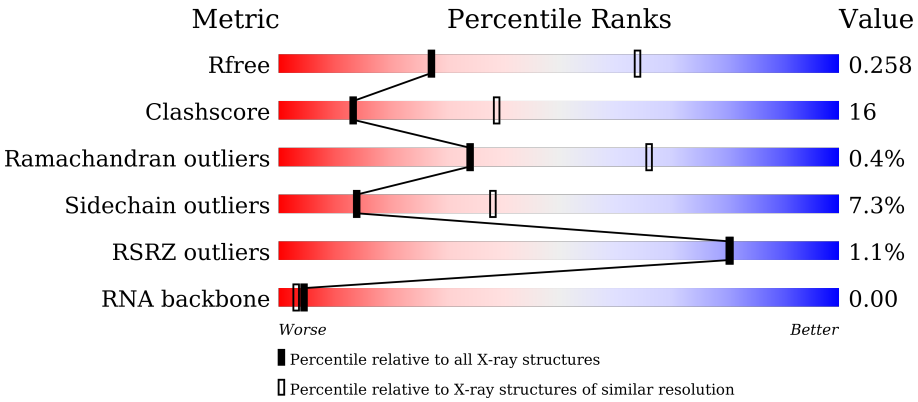
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.89 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))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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 <=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.

Mol	Chain	Length	Quality of chain
1	A	463	2% 60% 35%
1	B	463	66% 31%
2	C	4	25% 75%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7287 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 CRISPR system endoribonuclease Csm6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	0	0	0
			3573	2292	637	640	4			
1	B	462	Total	C	N	O	S	0	0	0
			3592	2306	640	642	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	161	ALA	TYR	engineered mutation	UNP Q53W17
B	161	ALA	TYR	engineered mutation	UNP Q53W17

- Molecule 2 is a RNA chain called RNA (5'-R(P*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	P	0	0	0
			88	40	20	24	4			

- Molecule 3 is water.

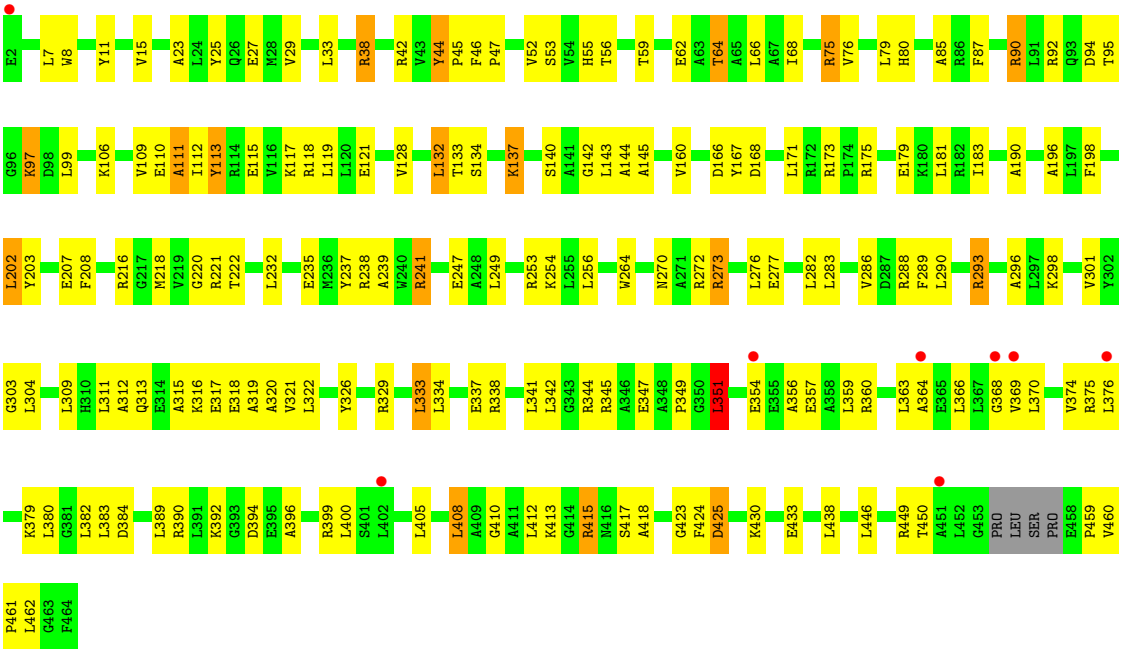
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total	O	0	0
			19	19		
3	B	15	Total	O	0	0
			15	15		

3 Residue-property plots (i)

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

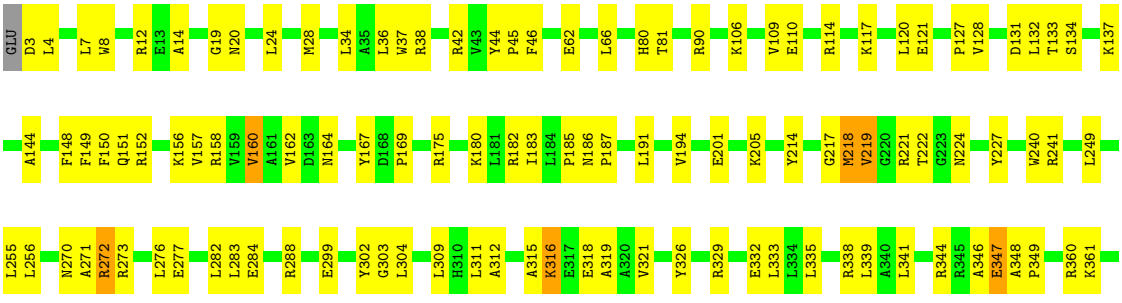
• Molecule 1: CRISPR system endoribonuclease Csm6

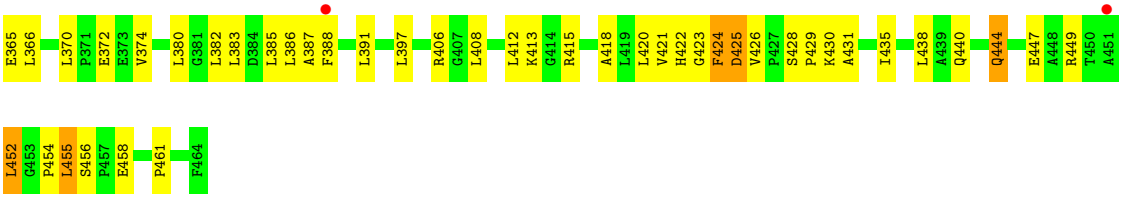
Chain A:



• Molecule 1: CRISPR system endoribonuclease Csm6

Chain B:





• Molecule 2: RNA (5'-R(P*AP*AP*AP*A)-3')

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	116.24Å 116.24Å 156.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.81 – 2.89 29.81 – 2.89	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.81-2.89) 100.0 (29.81-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 2.90Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.197 , 0.253 0.201 , 0.258	Depositor DCC
R_{free} test set	1999 reflections (8.10%)	wwPDB-VP
Wilson B-factor (Å^2)	68.0	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 35.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7287	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.50	0/3645	0.74	4/4937 (0.1%)
1	B	0.48	0/3667	0.71	1/4971 (0.0%)
2	C	1.09	0/99	1.84	3/152 (2.0%)
All	All	0.50	0/7411	0.76	8/10060 (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	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	A	C8-N9-C4	6.39	108.36	105.80
1	A	202	LEU	CA-CB-CG	6.29	129.76	115.30
1	B	218	MET	CB-CG-SD	-5.67	95.38	112.40
2	C	4	A	O5'-P-OP1	5.58	117.40	110.70
1	A	341	LEU	CA-CB-CG	5.44	127.81	115.30
2	C	3	A	O5'-P-OP2	-5.42	100.82	105.70
1	A	351	LEU	CA-CB-CG	5.20	127.27	115.30
1	A	333	LEU	CA-CB-CG	-5.14	103.48	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	417	SER	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	3573	0	3650	131	0
1	B	3592	0	3675	118	0
2	C	88	0	45	5	0
3	A	19	0	0	2	0
3	B	15	0	0	4	0
All	All	7287	0	7370	237	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 (237) 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:164:ASN:HD21	1:B:167:TYR:HB2	1.41	0.85
1:A:315:ALA:HB1	1:A:319:ALA:HB3	1.58	0.84
1:A:45:PRO:HG2	1:A:183:ILE:HG12	1.60	0.82
1:B:304:LEU:HD23	1:B:333:LEU:HD11	1.63	0.81
1:B:117:LYS:O	1:B:121:GLU:HG3	1.84	0.76
1:A:117:LYS:NZ	1:A:121:GLU:OE2	2.18	0.76
1:A:23:ALA:O	1:A:27:GLU:HG2	1.87	0.75
1:A:133:THR:O	1:B:137:LYS:NZ	2.19	0.75
1:A:238:ARG:NH1	1:B:318:GLU:O	2.21	0.74
1:A:273:ARG:NH1	1:A:277:GLU:OE2	2.21	0.73
1:B:455:LEU:HD13	1:B:456:SER:H	1.54	0.73
2:C:1:A:P	2:C:4:A:O3'	2.47	0.72
1:A:349:PRO:HG3	1:A:380:LEU:HG	1.72	0.71
1:B:299:GLU:HB3	1:B:452:LEU:HD21	1.72	0.71
1:A:115:GLU:OE2	1:A:118:ARG:NH2	2.24	0.70
1:A:304:LEU:HD23	1:A:333:LEU:HD22	1.72	0.70
1:A:75:ARG:HH11	1:A:75:ARG:HB3	1.56	0.70
1:B:110:GLU:O	1:B:114:ARG:HG3	1.92	0.69
1:B:339:LEU:HD22	1:B:346:ALA:HB2	1.74	0.69
1:B:382:LEU:HD23	1:B:412:LEU:HD11	1.74	0.69
1:A:396:ALA:HA	1:A:399:ARG:HH11	1.59	0.67
1:B:36:LEU:HD22	1:B:42:ARG:HH12	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ARG:HB3	1:A:75:ARG:NH1	2.10	0.66
1:B:256:LEU:HD11	1:B:277:GLU:HA	1.77	0.66
1:A:235:GLU:OE1	3:A:501:HOH:O	2.14	0.65
1:A:344:ARG:HH22	1:A:351:LEU:HA	1.61	0.65
1:A:357:GLU:HA	1:A:360:ARG:NH1	2.12	0.65
1:B:349:PRO:HG3	1:B:380:LEU:HG	1.79	0.65
1:A:408:LEU:O	1:A:412:LEU:HD12	1.96	0.65
1:A:338:ARG:NH2	1:A:394:ASP:OD1	2.30	0.64
1:B:151:GLN:NE2	1:B:157:VAL:O	2.30	0.64
1:B:44:TYR:HB3	1:B:45:PRO:HD3	1.79	0.64
1:B:382:LEU:HB3	1:B:412:LEU:HD11	1.78	0.64
1:A:334:LEU:O	1:A:338:ARG:HG2	1.99	0.63
1:A:337:GLU:OE2	1:A:449:ARG:NH2	2.32	0.63
1:A:62:GLU:OE2	1:A:62:GLU:N	2.25	0.63
1:A:418:ALA:N	1:A:425:ASP:OD1	2.32	0.62
1:A:196:ALA:HB2	1:A:218:MET:HE3	1.82	0.61
1:A:198:PHE:O	1:A:202:LEU:HD22	2.00	0.61
1:B:425:ASP:OD1	1:B:425:ASP:N	2.34	0.61
1:A:52:VAL:HB	1:A:128:VAL:HG22	1.82	0.61
1:B:117:LYS:HD2	1:B:150:PHE:CZ	2.34	0.61
1:A:109:VAL:HG23	1:A:142:GLY:HA2	1.82	0.60
1:B:127:PRO:HA	1:B:156:LYS:HB3	1.82	0.60
1:A:109:VAL:HG22	1:B:187:PRO:HG3	1.81	0.60
1:A:38:ARG:NH2	1:A:94:ASP:O	2.35	0.60
1:B:36:LEU:HD22	1:B:42:ARG:NH1	2.17	0.60
1:A:238:ARG:HD2	1:B:318:GLU:HB2	1.83	0.60
1:A:11:TYR:O	1:A:15:VAL:HG23	2.02	0.59
1:A:359:LEU:HB3	1:A:376:LEU:HD11	1.83	0.59
1:A:356:ALA:O	1:A:360:ARG:HG3	2.02	0.59
1:B:272:ARG:HG3	1:B:461:PRO:HD2	1.84	0.59
1:A:202:LEU:HB3	1:A:207:GLU:HB2	1.84	0.59
1:A:145:ALA:HB2	1:B:148:PHE:HD2	1.68	0.58
1:B:382:LEU:HB3	1:B:412:LEU:CD1	2.32	0.58
1:A:196:ALA:HB2	1:A:218:MET:CE	2.34	0.58
1:A:113:TYR:CG	1:B:187:PRO:HB3	2.38	0.58
1:B:241:ARG:HD3	1:B:311:LEU:HD21	1.86	0.58
1:A:166:ASP:OD2	1:A:175:ARG:NE	2.37	0.57
1:A:329:ARG:NH2	1:B:423:GLY:O	2.36	0.57
1:B:19:GLY:HA3	1:B:24:LEU:HD22	1.85	0.57
1:B:152:ARG:HD2	1:B:152:ARG:N	2.18	0.57
1:B:430:LYS:HG3	1:B:431:ALA:N	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:TYR:CE1	1:A:173:ARG:HD3	2.39	0.57
1:A:354:GLU:O	1:A:357:GLU:HG2	2.05	0.56
1:A:272:ARG:HG3	1:A:461:PRO:HD2	1.87	0.56
1:A:289:PHE:CZ	1:B:424:PHE:HZ	2.23	0.56
1:B:360:ARG:HG2	1:B:374:VAL:HB	1.88	0.56
1:B:302:TYR:CE1	1:B:447:GLU:HB2	2.40	0.55
1:B:428:SER:OG	1:B:430:LYS:HG2	2.05	0.55
1:B:447:GLU:OE2	1:B:454:PRO:HB3	2.07	0.55
1:A:137:LYS:NZ	1:B:133:THR:O	2.39	0.55
1:B:312:ALA:HB2	1:B:326:TYR:HB2	1.89	0.55
1:A:312:ALA:HB2	1:A:326:TYR:HB2	1.89	0.55
1:A:319:ALA:O	1:A:321:VAL:N	2.39	0.55
1:A:137:LYS:HD3	2:C:4:A:OP2	2.07	0.54
1:A:319:ALA:HB1	1:A:322:LEU:HB2	1.89	0.54
1:A:253:ARG:HG3	1:A:253:ARG:HH11	1.72	0.54
1:B:299:GLU:HA	1:B:452:LEU:HD11	1.90	0.54
1:B:3:ASP:CG	1:B:4:LEU:H	2.11	0.53
1:A:55:HIS:HB3	1:A:64:THR:HG22	1.90	0.53
1:B:271:ALA:O	1:B:272:ARG:HD3	2.07	0.53
1:B:270:ASN:HA	1:B:273:ARG:CG	2.38	0.53
1:A:56:THR:HG23	1:A:143:LEU:HD22	1.90	0.53
1:A:132:LEU:HB2	1:A:140:SER:HB3	1.91	0.53
1:A:286:VAL:HG13	1:A:304:LEU:HB2	1.90	0.53
1:B:270:ASN:OD1	1:B:273:ARG:HD2	2.09	0.53
1:B:347:GLU:HG2	1:B:348:ALA:N	2.24	0.52
1:A:232:LEU:O	1:A:235:GLU:HB3	2.09	0.52
1:B:372:GLU:H	1:B:372:GLU:CD	2.12	0.52
1:A:423:GLY:O	1:B:329:ARG:NH2	2.32	0.52
1:B:240:TRP:CD2	1:B:283:LEU:HD21	2.45	0.52
1:B:255:LEU:HD21	1:B:276:LEU:HD21	1.90	0.52
1:B:249:LEU:HD22	1:B:284:GLU:HA	1.92	0.52
1:B:321:VAL:HG12	1:B:426:VAL:HG23	1.92	0.52
1:B:418:ALA:HB3	1:B:421:VAL:HG23	1.92	0.52
1:A:117:LYS:HD2	1:B:194:VAL:HG12	1.92	0.52
1:B:315:ALA:HB1	1:B:319:ALA:HB3	1.91	0.51
1:B:151:GLN:OE1	1:B:186:ASN:HB2	2.10	0.51
1:A:383:LEU:HD13	1:A:412:LEU:HD13	1.93	0.51
1:B:372:GLU:OE1	1:B:372:GLU:N	2.33	0.50
1:A:132:LEU:HD22	1:A:144:ALA:HB2	1.94	0.50
1:A:293:ARG:HG2	1:A:293:ARG:HH11	1.76	0.50
1:A:364:ALA:O	1:A:368:GLY:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:LEU:HG	1:A:412:LEU:HD23	1.93	0.50
1:B:440:GLN:O	1:B:444:GLN:HG3	2.12	0.49
1:B:270:ASN:HA	1:B:273:ARG:HG3	1.94	0.49
1:B:37:TRP:CD2	1:B:66:LEU:HD22	2.48	0.49
1:B:408:LEU:HD13	1:B:438:LEU:HD22	1.95	0.49
1:A:25:TYR:CE1	1:A:29:VAL:HG11	2.47	0.49
1:A:413:LYS:HD2	1:A:413:LYS:O	2.13	0.49
1:B:20:ASN:O	1:B:24:LEU:HB2	2.13	0.49
1:B:412:LEU:CD2	1:B:435:ILE:HD11	2.43	0.49
1:B:222:THR:O	1:B:224:ASN:N	2.45	0.48
1:B:413:LYS:HE2	1:B:413:LYS:HA	1.95	0.48
1:A:167:TYR:CE2	2:C:2:A:H2'	2.47	0.48
1:B:201:GLU:O	1:B:205:LYS:HG2	2.13	0.48
1:A:203:TYR:HH	1:A:237:TYR:HE2	1.61	0.48
1:A:282:LEU:O	1:A:286:VAL:HG23	2.14	0.48
1:A:80:HIS:CE1	1:A:85:ALA:HB2	2.49	0.48
1:A:110:GLU:O	1:A:111:ALA:HB2	2.14	0.47
1:B:282:LEU:HD11	1:B:303:GLY:CA	2.45	0.47
1:B:137:LYS:HG2	2:C:2:A:OP2	2.14	0.47
1:A:270:ASN:OD1	1:A:273:ARG:HD3	2.14	0.47
1:A:256:LEU:HD22	1:A:273:ARG:NH1	2.30	0.47
1:B:8:TRP:CD1	1:B:175:ARG:HG3	2.49	0.47
1:B:151:GLN:OE1	1:B:186:ASN:ND2	2.45	0.47
1:B:339:LEU:HD11	1:B:388:PHE:CE2	2.49	0.47
1:A:113:TYR:HD2	1:B:191:LEU:HD12	1.79	0.47
1:A:115:GLU:O	1:A:119:LEU:HG	2.14	0.47
1:A:203:TYR:CE2	1:A:462:LEU:HD21	2.49	0.47
1:A:329:ARG:HD2	1:A:329:ARG:HA	1.74	0.47
1:B:152:ARG:HD2	1:B:152:ARG:H	1.78	0.47
1:B:80:HIS:HD2	1:B:81:THR:O	1.98	0.46
1:A:239:ALA:HB1	1:A:247:GLU:HB3	1.97	0.46
1:A:318:GLU:HG2	1:A:319:ALA:N	2.30	0.46
1:A:90:ARG:HD3	1:A:90:ARG:N	2.30	0.46
1:A:59:THR:HA	1:A:87:PHE:CE2	2.51	0.46
1:A:363:LEU:HB2	1:A:374:VAL:HG11	1.96	0.46
1:B:341:LEU:HD11	1:B:449:ARG:NH1	2.31	0.46
1:B:366:LEU:HD23	1:B:383:LEU:HD11	1.97	0.46
1:A:208:PHE:HZ	1:A:459:PRO:HG3	1.81	0.46
1:A:338:ARG:NH2	1:A:396:ALA:HB3	2.31	0.46
1:A:364:ALA:HB1	1:A:369:VAL:O	2.16	0.46
1:B:8:TRP:NE1	1:B:12:ARG:HD2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:LEU:H	1:B:415:ARG:NH2	2.14	0.46
1:A:109:VAL:HG23	1:A:142:GLY:CA	2.45	0.45
1:A:8:TRP:CZ2	1:A:175:ARG:HA	2.51	0.45
1:A:33:LEU:HD22	1:A:66:LEU:HD21	1.97	0.45
1:B:346:ALA:O	1:B:347:GLU:HB3	2.16	0.45
1:A:92:ARG:HG3	1:A:99:LEU:HD12	1.98	0.45
1:B:134:SER:OG	2:C:3:A:OP2	2.33	0.45
1:A:264:TRP:O	1:A:270:ASN:ND2	2.49	0.45
1:A:410:GLY:O	1:A:413:LYS:HB3	2.17	0.45
1:A:241:ARG:HB3	1:A:311:LEU:HD21	1.99	0.45
1:A:366:LEU:HD21	1:A:405:LEU:HB3	1.99	0.45
1:A:168:ASP:HB3	1:A:171:LEU:HB2	1.97	0.45
1:B:256:LEU:HA	1:B:256:LEU:HD23	1.71	0.45
1:A:76:VAL:HG21	1:A:97:LYS:HE3	1.98	0.45
1:A:232:LEU:HD21	1:A:254:LYS:HB3	1.98	0.45
1:B:372:GLU:CD	1:B:372:GLU:N	2.71	0.45
1:B:62:GLU:HG3	1:B:90:ARG:HH21	1.82	0.44
1:B:421:VAL:HG12	1:B:422:HIS:H	1.82	0.44
1:B:276:LEU:HD12	1:B:276:LEU:HA	1.80	0.44
1:A:220:GLY:HA2	3:A:503:HOH:O	2.18	0.44
1:A:46:PHE:CD1	1:A:47:PRO:HD2	2.52	0.44
1:A:79:LEU:HD23	1:A:112:ILE:HD13	1.99	0.44
1:B:7:LEU:HD12	1:B:7:LEU:HA	1.78	0.44
1:A:132:LEU:CD2	1:A:144:ALA:HB2	2.48	0.44
1:A:62:GLU:H	1:A:62:GLU:CD	2.17	0.44
1:B:158:ARG:NH2	3:B:502:HOH:O	2.40	0.44
1:A:446:LEU:O	1:A:450:THR:HG23	2.18	0.44
1:B:272:ARG:HD2	1:B:272:ARG:HA	1.77	0.44
1:A:44:TYR:CG	1:A:45:PRO:N	2.85	0.43
1:A:87:PHE:HA	1:A:90:ARG:HG2	2.00	0.43
1:A:59:THR:HB	1:B:169:PRO:HB3	2.00	0.43
1:B:214:TYR:O	1:B:218:MET:HG2	2.18	0.43
1:A:301:VAL:HG11	1:A:337:GLU:HB2	2.00	0.43
1:A:290:LEU:HD21	1:A:304:LEU:CD1	2.49	0.43
1:A:347:GLU:O	1:A:379:LYS:HG2	2.19	0.43
1:A:382:LEU:HD12	1:A:382:LEU:HA	1.69	0.43
1:B:191:LEU:HD23	1:B:191:LEU:HA	1.76	0.43
1:B:128:VAL:HB	1:B:157:VAL:HG22	2.01	0.43
1:B:185:PRO:HA	3:B:502:HOH:O	2.18	0.43
1:A:68:ILE:HD12	1:A:95:THR:HG21	1.99	0.43
1:B:316:LYS:NZ	1:B:429:PRO:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:ALA:O	1:B:391:LEU:HD13	2.19	0.43
1:A:390:ARG:CD	1:A:405:LEU:HD11	2.49	0.43
1:B:14:ALA:HB1	1:B:24:LEU:HD21	2.01	0.43
1:A:190:ALA:O	1:A:222:THR:HG22	2.19	0.43
1:A:316:LYS:NZ	1:A:433:GLU:OE2	2.41	0.42
1:A:389:LEU:HD22	1:A:394:ASP:OD2	2.19	0.42
1:B:435:ILE:HD13	1:B:435:ILE:HA	1.72	0.42
1:B:282:LEU:HD11	1:B:303:GLY:HA3	2.00	0.42
1:B:447:GLU:C	1:B:449:ARG:H	2.22	0.42
1:A:53:SER:HB2	1:A:55:HIS:NE2	2.35	0.42
1:B:339:LEU:HD22	1:B:385:LEU:HD11	2.01	0.42
1:B:332:GLU:HA	1:B:382:LEU:HD11	2.00	0.42
1:B:149:PHE:O	1:B:152:ARG:HG2	2.19	0.42
1:B:256:LEU:HD22	1:B:273:ARG:NH2	2.34	0.42
1:A:55:HIS:CD2	1:A:55:HIS:N	2.87	0.42
1:A:276:LEU:HD21	1:A:460:VAL:HG21	2.01	0.42
1:A:319:ALA:O	1:A:322:LEU:N	2.48	0.42
1:B:397:LEU:HA	1:B:397:LEU:HD23	1.85	0.42
1:A:400:LEU:HD11	1:A:438:LEU:HD11	2.01	0.42
1:A:382:LEU:H	1:A:415:ARG:HH22	1.68	0.41
1:A:112:ILE:HG21	1:A:143:LEU:N	2.35	0.41
1:A:283:LEU:HD23	1:A:283:LEU:HA	1.93	0.41
1:B:34:LEU:O	1:B:38:ARG:HG3	2.20	0.41
1:B:37:TRP:CZ2	1:B:42:ARG:HB2	2.55	0.41
1:B:133:THR:HG21	1:B:162:VAL:HB	2.02	0.41
1:B:335:LEU:HD23	1:B:335:LEU:HA	1.80	0.41
1:A:7:LEU:HD12	1:A:7:LEU:HA	1.90	0.41
1:A:42:ARG:NH2	1:A:179:GLU:O	2.45	0.41
1:A:160:VAL:HG23	1:A:181:LEU:HD11	2.01	0.41
1:B:132:LEU:HD22	1:B:144:ALA:HB2	2.02	0.41
1:B:182:ARG:NH2	3:B:501:HOH:O	2.34	0.41
1:A:45:PRO:HG2	1:A:183:ILE:CG1	2.42	0.41
1:A:55:HIS:CE1	1:A:68:ILE:HG12	2.55	0.41
1:B:219:VAL:HG12	1:B:227:TYR:HB2	2.03	0.41
1:A:296:ALA:O	1:A:298:LYS:N	2.53	0.41
1:A:313:GLN:O	1:A:316:LYS:HG2	2.20	0.41
1:A:392:LYS:HA	1:A:392:LYS:HD2	1.87	0.41
1:A:52:VAL:O	1:A:128:VAL:HA	2.20	0.41
1:A:76:VAL:CG2	1:A:97:LYS:HE3	2.51	0.41
1:B:120:LEU:HD13	1:B:157:VAL:HG21	2.01	0.41
1:A:282:LEU:HD11	1:A:303:GLY:HA3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:ASP:HA	1:B:160:VAL:HG22	2.03	0.40
1:B:309:LEU:HD23	1:B:309:LEU:HA	1.90	0.40
1:A:237:TYR:OH	1:A:460:VAL:HG13	2.21	0.40
1:B:109:VAL:N	3:B:503:HOH:O	2.53	0.40
1:B:137:LYS:HA	1:B:137:LYS:HD3	1.82	0.40
1:B:183:ILE:H	1:B:183:ILE:HG12	1.74	0.40
1:B:456:SER:OG	1:B:458:GLU:HG3	2.21	0.40
1:A:253:ARG:HG3	1:A:253:ARG:NH1	2.36	0.40
1:B:217:GLY:O	1:B:221:ARG:N	2.50	0.40
1:B:420:LEU:HA	1:B:420:LEU:HD23	1.83	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	455/463 (98%)	432 (95%)	21 (5%)	2 (0%)	34	66
1	B	460/463 (99%)	434 (94%)	24 (5%)	2 (0%)	34	66
All	All	915/926 (99%)	866 (95%)	45 (5%)	4 (0%)	34	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	320	ALA
1	A	111	ALA
1	B	347	GLU
1	B	46	PHE

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	350/354 (99%)	319 (91%)	31 (9%)	9 29
1	B	353/354 (100%)	333 (94%)	20 (6%)	20 51
All	All	703/708 (99%)	652 (93%)	51 (7%)	14 38

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	44	TYR
1	A	64	THR
1	A	75	ARG
1	A	90	ARG
1	A	97	LYS
1	A	106	LYS
1	A	113	TYR
1	A	132	LEU
1	A	134	SER
1	A	137	LYS
1	A	216	ARG
1	A	221	ARG
1	A	241	ARG
1	A	249	LEU
1	A	273	ARG
1	A	288	ARG
1	A	293	ARG
1	A	309	LEU
1	A	317	GLU
1	A	342	LEU
1	A	345	ARG
1	A	351	LEU
1	A	370	LEU
1	A	375	ARG
1	A	384	ASP
1	A	408	LEU

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Mol	Chain	Res	Type
1	A	415	ARG
1	A	424	PHE
1	A	425	ASP
1	A	430	LYS
1	B	28	MET
1	B	106	LYS
1	B	160	VAL
1	B	180	LYS
1	B	219	VAL
1	B	272	ARG
1	B	288	ARG
1	B	316	LYS
1	B	338	ARG
1	B	344	ARG
1	B	361	LYS
1	B	365	GLU
1	B	370	LEU
1	B	386	LEU
1	B	406	ARG
1	B	424	PHE
1	B	425	ASP
1	B	444	GLN
1	B	452	LEU
1	B	455	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	26	GLN
1	B	80	HIS
1	B	164	ASN
1	B	444	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	3/4 (75%)	3 (100%)	1 (33%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	2	A
2	C	3	A
2	C	4	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	2	A

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 monosaccharides 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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	459/463 (99%)	0.07	8 (1%) 70 69	41, 63, 89, 102	0
1	B	462/463 (99%)	0.01	2 (0%) 92 93	38, 67, 90, 111	0
2	C	4/4 (100%)	1.38	0 100 100	46, 49, 49, 54	0
All	All	925/930 (99%)	0.05	10 (1%) 80 80	38, 65, 89, 111	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	451	ALA	3.4
1	A	368	GLY	3.1
1	A	364	ALA	2.5
1	A	402	LEU	2.4
1	A	376	LEU	2.3
1	A	369	VAL	2.2
1	A	354	GLU	2.2
1	A	451	ALA	2.2
1	B	388	PHE	2.2
1	A	2	GLU	2.1

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.