



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:34 AM GMT

PDB ID : 2R9Q
Title : Crystal structure of 2'-deoxycytidine 5'-triphosphate deaminase from *Agrobacterium tumefaciens*
Authors : Zhang, R.; Dong, A.; Xu, X.; Savchenko, A.; Edwards, A.M.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2007-09-13
Resolution : 2.20 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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

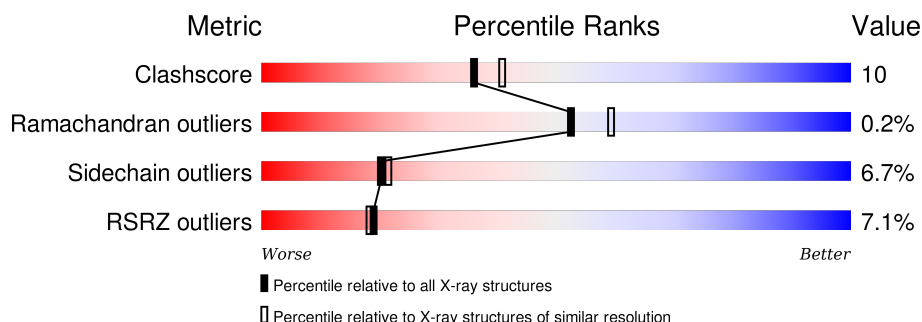
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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 $\leq 5\%$. 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	370	<div> <div>6%</div> <div> <div></div> <div>71%</div> <div>16%</div> <div>•</div> <div>12%</div> </div> </div>
1	B	370	<div> <div>9%</div> <div> <div></div> <div>71%</div> <div>19%</div> <div>•</div> <div>8%</div> </div> </div>
1	C	370	<div> <div>4%</div> <div> <div></div> <div>68%</div> <div>19%</div> <div>•</div> <div>11%</div> </div> </div>
1	D	370	<div> <div>6%</div> <div> <div></div> <div>69%</div> <div>17%</div> <div>•</div> <div>11%</div> </div> </div>
2	X	7	<div> <div>29%</div> <div> <div></div> <div>71%</div> <div>14%</div> <div></div> <div>14%</div> </div> </div>
3	Y	9	<div> <div></div> <div> <div></div> <div>56%</div> <div>33%</div> <div></div> <div>11%</div> </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10768 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 2'-deoxycytidine 5'-triphosphate deaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2478	1590	426	455	7			
1	B	342	Total	C	N	O	S	0	0	0
			2607	1664	456	480	7			
1	C	331	Total	C	N	O	S	0	0	0
			2493	1591	433	462	7			
1	D	330	Total	C	N	O	S	0	0	0
			2465	1584	425	449	7			

- Molecule 2 is a protein called Synthetic peptide 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	7	Total	C	N	O	S	0	0	0
			44	26	8	9	1			

- Molecule 3 is a protein called Synthetic peptide 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Y	9	Total	C	N	O	0	0	0
			59	39	9	11			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	152	Total	O	0	0
			152	152		
4	B	170	Total	O	0	0
			170	170		
4	C	138	Total	O	0	0
			138	138		
4	D	157	Total	O	0	0
			157	157		

Continued on next page...

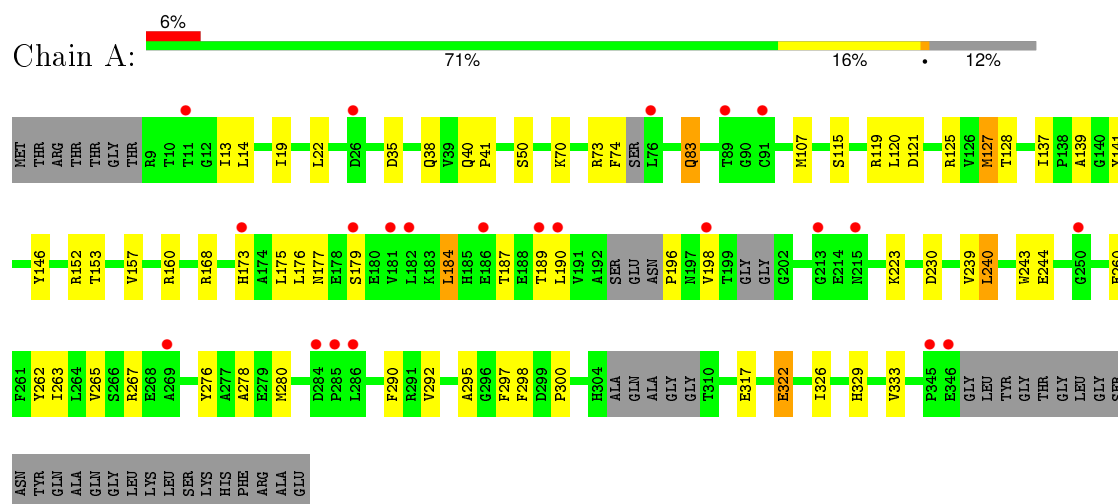
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	X	1	Total	O	0	0
			1	1		
4	Y	4	Total	O	0	0
			4	4		

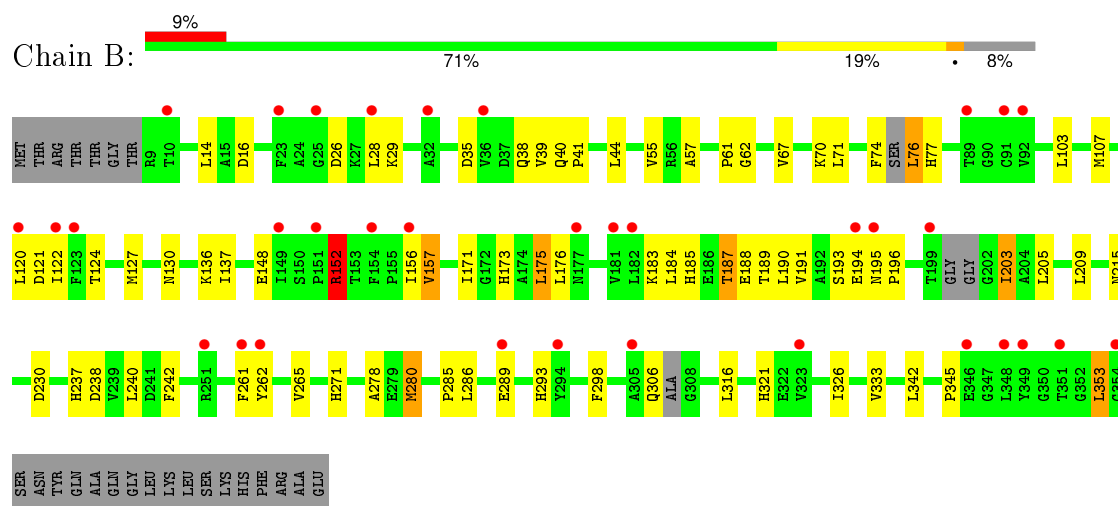
3 Residue-property plots [i](#)

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.

- Molecule 1: 2'-deoxycytidine 5'-triphosphate deaminase

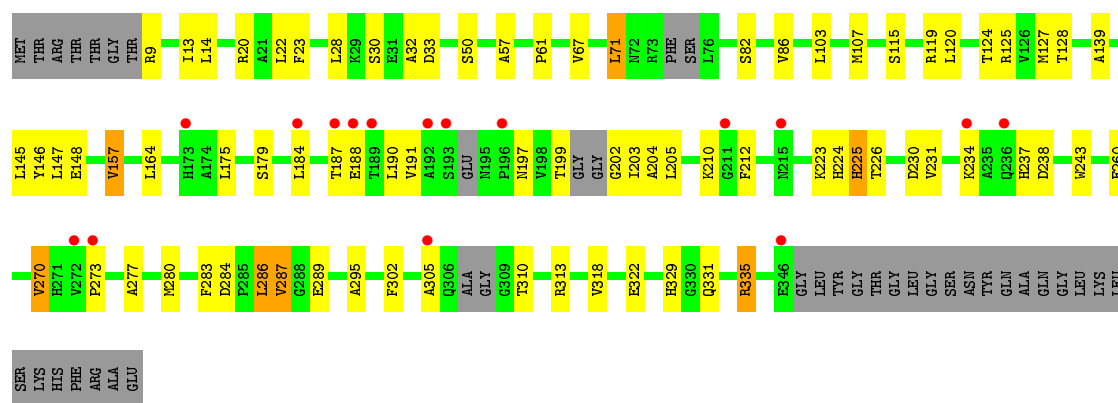


- Molecule 1: 2'-deoxycytidine 5'-triphosphate deaminase

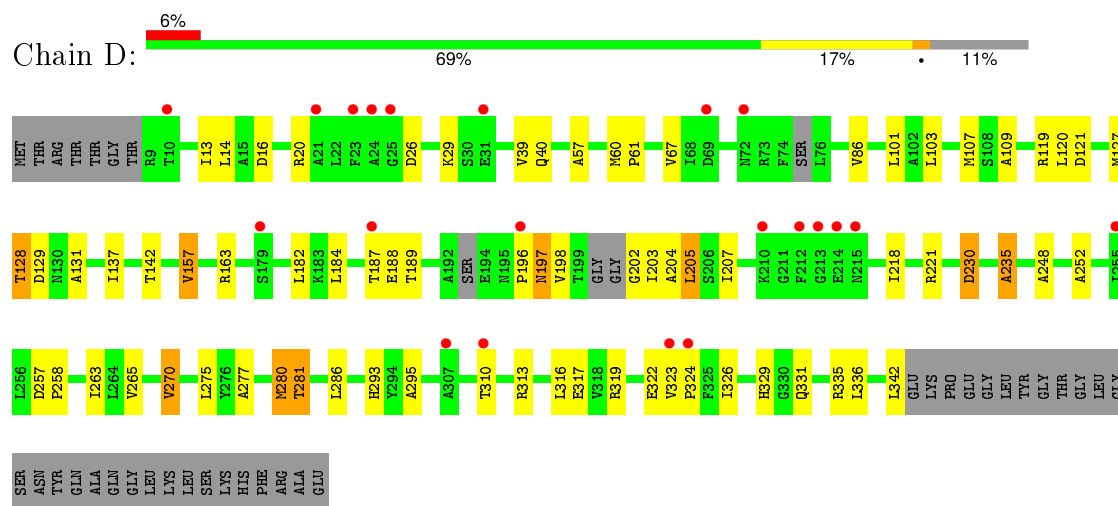


- Molecule 1: 2'-deoxycytidine 5'-triphosphate deaminase

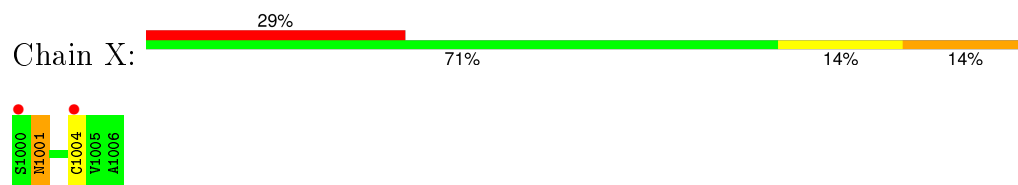




- Molecule 1: 2'-deoxycytidine 5'-triphosphate deaminase



- Molecule 2: Synthetic peptide 1



- Molecule 3: Synthetic peptide 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.69 Å 129.04 Å 85.56 Å 90.00° 108.75° 90.00°	Depositor
Resolution (Å)	46.78 – 2.20 46.77 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.9 (46.78-2.20) 93.9 (46.77-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.20 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.189 , 0.269 0.185 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 69790 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10768	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.69	0/2531	0.74	1/3434 (0.0%)
1	B	0.73	0/2663	0.82	2/3609 (0.1%)
1	C	0.78	2/2545 (0.1%)	0.83	6/3457 (0.2%)
1	D	0.67	0/2520	0.76	3/3428 (0.1%)
2	X	0.63	0/44	0.91	0/60
3	Y	0.67	0/59	0.67	0/81
All	All	0.72	2/10362 (0.0%)	0.79	12/14069 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	289	GLU	CB-CG	9.51	1.70	1.52
1	C	289	GLU	CG-CD	6.28	1.61	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	20	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	B	152	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	C	20	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	C	125	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	C	335	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	D	163	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	D	163	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	C	335	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	C	33	ASP	CB-CG-OD1	5.31	123.08	118.30
1	D	230	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	121	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	125	ARG	NE-CZ-NH1	5.20	122.90	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2478	0	2427	45	0
1	B	2607	0	2571	53	0
1	C	2493	0	2427	51	0
1	D	2465	0	2388	46	0
2	X	44	0	41	2	0
3	Y	59	0	63	1	0
4	A	152	0	0	2	0
4	B	170	0	0	3	0
4	C	138	0	0	9	0
4	D	157	0	0	8	0
4	X	1	0	0	0	0
4	Y	4	0	0	0	0
All	All	10768	0	9917	192	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 10.

All (192) 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:A:260:GLU:OE1	1:A:262:TYR:OH	1.80	0.99
1:C:184:LEU:HD22	1:C:190:LEU:HD21	1.47	0.94
1:B:205:LEU:HD12	1:B:280:MET:CE	2.06	0.86
1:B:286:LEU:HD22	1:B:289:GLU:OE1	1.77	0.82
1:D:128:THR:HG22	1:D:131:ALA:HB2	1.59	0.82
1:C:184:LEU:HD21	1:C:273:PRO:HG2	1.63	0.80
1:B:152:ARG:HD3	1:D:322:GLU:OE1	1.83	0.79
1:B:289:GLU:HG3	4:D:382:HOH:O	1.84	0.78
1:C:287:VAL:HG12	4:C:504:HOH:O	1.82	0.78
1:A:322:GLU:N	4:A:523:HOH:O	2.06	0.75
1:B:173:HIS:CE1	1:B:175:LEU:HD21	2.21	0.75
1:C:184:LEU:CD2	1:C:190:LEU:HD21	2.18	0.73
1:A:243:TRP:CH2	1:A:263:ILE:HD11	2.25	0.72
1:B:152:ARG:HH11	1:B:152:ARG:HG3	1.53	0.71
1:B:205:LEU:HD12	1:B:280:MET:HE3	1.71	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:LEU:HD12	1:B:280:MET:HE1	1.71	0.71
1:C:157:VAL:HG13	1:C:230:ASP:HA	1.72	0.71
1:B:171:ILE:HD12	1:B:342:LEU:HD11	1.71	0.71
1:C:67:VAL:HG12	1:C:71:LEU:CD2	2.22	0.70
1:B:289:GLU:OE2	1:D:60:MET:HE1	1.93	0.69
1:A:223:LYS:HE3	1:A:244:GLU:HG3	1.75	0.68
1:C:199:THR:HG22	4:C:437:HOH:O	1.95	0.67
1:D:157:VAL:HG13	1:D:230:ASP:HA	1.78	0.66
1:C:210:LYS:HG2	1:C:329:HIS:CE1	2.32	0.65
1:D:14:LEU:HD21	1:D:107:MET:CE	2.26	0.65
1:A:196:PRO:O	1:A:198:VAL:HG23	1.97	0.65
1:B:195:ASN:HB2	1:B:196:PRO:HD2	1.78	0.65
1:D:280:MET:HB3	1:D:295:ALA:HB1	1.80	0.64
1:B:77:HIS:HB2	4:B:495:HOH:O	1.95	0.64
1:C:191:VAL:CG2	1:C:203:ILE:HD12	2.28	0.64
1:D:197:ASN:HB3	1:D:204:ALA:HB3	1.81	0.63
1:D:205:LEU:HD23	1:D:280:MET:HE2	1.81	0.62
3:Y:1019:VAL:HG13	3:Y:1020:PRO:HD2	1.81	0.62
1:D:263:ILE:HD13	1:D:317:GLU:HG3	1.81	0.62
1:A:184:LEU:HD13	1:A:190:LEU:HD21	1.81	0.62
1:C:184:LEU:HD22	1:C:190:LEU:CD2	2.24	0.61
1:B:289:GLU:OE2	1:D:60:MET:CE	2.48	0.61
1:A:14:LEU:HD21	1:A:107:MET:HE1	1.82	0.61
1:B:262:TYR:OH	4:B:541:HOH:O	2.12	0.60
1:B:157:VAL:HG13	1:B:230:ASP:HA	1.84	0.58
1:A:127:MET:HG3	1:A:146:TYR:HB2	1.84	0.58
1:D:196:PRO:HB2	1:D:203:ILE:HD12	1.86	0.58
1:B:183:LYS:O	1:B:187:THR:HG22	2.02	0.58
1:A:83:GLN:HA	1:A:83:GLN:HE21	1.67	0.57
1:D:207:ILE:HD12	4:D:525:HOH:O	2.04	0.57
1:A:177:ASN:OD1	1:A:179:SER:HB3	2.04	0.57
1:D:218:ILE:HD13	1:D:248:ALA:N	2.19	0.57
1:D:316:LEU:HD12	4:D:525:HOH:O	2.04	0.57
1:B:345:PRO:HB2	1:B:353:LEU:HG	1.87	0.57
1:A:267:ARG:HD3	1:A:329:HIS:CE1	2.39	0.57
1:B:28:LEU:HD21	1:B:44:LEU:HD22	1.87	0.56
1:B:152:ARG:HG3	1:B:152:ARG:NH1	2.20	0.56
1:D:182:LEU:HG	1:D:198:VAL:HG21	1.87	0.56
1:D:202:GLY:N	4:D:406:HOH:O	2.39	0.56
1:A:119:ARG:HD3	1:A:317:GLU:OE2	2.06	0.56
1:A:239:VAL:HG23	1:A:240:LEU:HD13	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:ILE:HG13	1:D:57:ALA:HB3	1.89	0.55
1:D:128:THR:HG23	1:D:129:ASP:O	2.06	0.55
1:A:157:VAL:HG13	1:A:230:ASP:HA	1.88	0.55
1:C:13:ILE:HD13	1:C:277:ALA:HB3	1.89	0.55
1:D:14:LEU:HD21	1:D:107:MET:HE1	1.88	0.55
1:B:293:HIS:NE2	1:B:321:HIS:CE1	2.75	0.55
1:D:121:ASP:OD2	1:D:319:ARG:NH2	2.39	0.54
1:C:67:VAL:HG12	1:C:71:LEU:HD23	1.90	0.54
1:A:290:PHE:CE2	1:A:333:VAL:HG12	2.43	0.54
1:A:173:HIS:CE1	1:A:175:LEU:HD21	2.42	0.54
1:C:107:MET:O	1:C:139:ALA:HA	2.08	0.53
1:C:128:THR:HG22	1:C:145:LEU:HD23	1.89	0.53
1:C:13:ILE:CD1	1:C:277:ALA:HB3	2.39	0.53
1:C:61:PRO:HG3	1:C:127:MET:CE	2.39	0.52
1:D:270:VAL:HG11	1:D:336:LEU:HD22	1.91	0.52
1:A:128:THR:HG21	1:A:137:ILE:HG13	1.91	0.52
1:A:13:ILE:HD13	1:A:168:ARG:HD3	1.90	0.52
1:A:243:TRP:CH2	1:A:263:ILE:CD1	2.91	0.52
1:C:124:THR:HA	1:C:148:GLU:O	2.10	0.52
1:C:67:VAL:HG13	1:C:127:MET:HE1	1.93	0.51
1:C:212:PHE:HE2	1:C:313:ARG:HH12	1.59	0.51
1:B:185:HIS:O	1:B:188:GLU:O	2.29	0.51
1:A:326:ILE:HG13	1:C:57:ALA:HB3	1.93	0.51
1:B:191:VAL:CG2	1:B:203:ILE:HD13	2.41	0.51
1:C:283:PHE:CE2	1:C:286:LEU:HD12	2.45	0.51
1:B:184:LEU:HA	1:B:187:THR:CG2	2.40	0.51
1:D:61:PRO:HG3	1:D:127:MET:HE3	1.93	0.51
1:C:283:PHE:HE2	1:C:286:LEU:HD12	1.76	0.51
1:D:235:ALA:HB3	4:D:457:HOH:O	2.11	0.51
1:D:293:HIS:CE1	1:D:319:ARG:HB2	2.46	0.50
1:C:224:HIS:CD2	1:C:260:GLU:OE2	2.64	0.50
1:D:16:ASP:OD2	1:D:20:ARG:NH2	2.44	0.50
1:B:137:ILE:N	1:B:137:ILE:HD12	2.27	0.50
1:D:109:ALA:HB3	1:D:137:ILE:HB	1.94	0.50
1:D:316:LEU:HB2	4:D:525:HOH:O	2.12	0.50
1:D:265:VAL:CG2	1:D:313:ARG:HB3	2.42	0.50
1:C:237:HIS:NE2	4:C:500:HOH:O	2.27	0.49
1:C:115:SER:O	1:C:119:ARG:HG2	2.12	0.49
1:C:280:MET:O	1:C:295:ALA:HB1	2.11	0.49
1:B:316:LEU:HD13	1:B:333:VAL:HG21	1.94	0.49
1:A:243:TRP:CZ3	1:A:263:ILE:HD12	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ILE:HD13	1:B:156:ILE:HD13	1.95	0.49
1:C:202:GLY:N	4:C:414:HOH:O	2.45	0.49
1:A:176:LEU:HD21	1:A:276:TYR:CE1	2.48	0.49
1:C:199:THR:CG2	1:C:335:ARG:HD2	2.42	0.48
1:A:128:THR:HB	1:A:141:TYR:CZ	2.47	0.48
1:B:67:VAL:HG22	1:B:127:MET:HE2	1.94	0.48
1:A:184:LEU:HD22	1:A:184:LEU:O	2.14	0.48
1:B:55:VAL:HG12	1:B:76:LEU:CD2	2.44	0.48
1:D:67:VAL:HG13	1:D:127:MET:HE1	1.94	0.48
1:A:19:ILE:HA	1:A:22:LEU:HD12	1.95	0.48
1:C:231:VAL:O	1:C:234:LYS:HE2	2.13	0.48
1:A:40:GLN:HB3	1:A:41:PRO:HD2	1.96	0.48
1:A:280:MET:CE	1:A:292:VAL:HG11	2.44	0.48
1:C:226:THR:N	4:C:495:HOH:O	2.45	0.47
1:D:13:ILE:HD12	1:D:277:ALA:HB3	1.96	0.47
1:C:124:THR:HB	1:C:147:LEU:HD11	1.95	0.47
1:A:121:ASP:OD2	1:A:153:THR:OG1	2.25	0.47
1:D:16:ASP:HB3	1:D:40:GLN:O	2.15	0.47
2:X:1001:ASN:ND2	2:X:1001:ASN:C	2.68	0.47
1:A:137:ILE:N	1:A:137:ILE:HD12	2.29	0.47
1:C:14:LEU:HD21	1:C:107:MET:HE1	1.96	0.46
1:D:207:ILE:CD1	4:D:525:HOH:O	2.62	0.46
1:A:280:MET:O	1:A:295:ALA:HB1	2.15	0.46
1:C:23:PHE:HB2	1:C:28:LEU:HD23	1.97	0.46
1:A:265:VAL:HG22	4:A:519:HOH:O	2.15	0.46
1:C:184:LEU:HD21	1:C:273:PRO:CG	2.42	0.46
1:A:121:ASP:O	1:A:152:ARG:HB2	2.16	0.46
1:D:14:LEU:HD21	1:D:107:MET:HE2	1.98	0.46
1:B:61:PRO:HG3	1:B:127:MET:CE	2.46	0.46
1:C:9:ARG:N	4:C:388:HOH:O	2.49	0.45
1:A:223:LYS:HE3	1:A:244:GLU:CG	2.45	0.45
1:D:16:ASP:HB2	1:D:39:VAL:HG12	1.97	0.45
1:A:176:LEU:HD12	1:A:176:LEU:N	2.31	0.45
1:D:184:LEU:O	1:D:188:GLU:O	2.34	0.45
1:D:221:ARG:NH1	4:D:518:HOH:O	2.49	0.45
1:B:61:PRO:HG3	1:B:127:MET:HE3	1.99	0.45
1:B:293:HIS:NE2	1:B:321:HIS:HE1	2.14	0.45
1:D:189:THR:HB	1:D:310:THR:HG21	1.99	0.45
1:B:124:THR:HA	1:B:148:GLU:O	2.16	0.45
1:D:323:VAL:HG12	1:D:324:PRO:O	2.17	0.45
1:A:107:MET:O	1:A:139:ALA:HA	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:GLY:O	1:B:130:ASN:HA	2.17	0.44
1:A:128:THR:CG2	1:A:137:ILE:HG13	2.47	0.44
1:A:50:SER:OG	1:A:160:ARG:HD2	2.18	0.44
1:B:136:LYS:NZ	4:B:474:HOH:O	2.48	0.44
1:B:35:ASP:HB2	1:B:38:GLN:HB2	2.00	0.44
1:D:342:LEU:HA	1:D:342:LEU:HD23	1.83	0.44
1:C:184:LEU:O	1:C:188:GLU:O	2.35	0.44
1:B:74:PHE:CB	1:B:76:LEU:HD23	2.48	0.44
1:C:270:VAL:HG12	1:C:302:PHE:CE2	2.53	0.43
1:A:243:TRP:CZ3	1:A:263:ILE:CD1	3.02	0.43
1:A:115:SER:O	1:A:119:ARG:HG2	2.18	0.43
1:B:185:HIS:HD2	1:B:190:LEU:H	1.66	0.43
1:A:157:VAL:CG1	1:A:230:ASP:HA	2.48	0.43
1:C:270:VAL:HG12	1:C:302:PHE:HE2	1.83	0.43
1:C:199:THR:HG23	1:C:335:ARG:HD2	1.99	0.43
1:D:286:LEU:HD12	1:D:331:GLN:NE2	2.33	0.43
1:B:16:ASP:HB3	1:B:39:VAL:HG12	2.00	0.43
1:B:55:VAL:HG12	1:B:76:LEU:HD21	2.01	0.43
1:B:67:VAL:HG13	1:B:127:MET:HE1	2.01	0.43
1:C:164:LEU:N	1:C:164:LEU:HD12	2.34	0.42
1:A:35:ASP:HB2	1:A:38:GLN:HB2	2.00	0.42
1:B:57:ALA:HB3	1:D:326:ILE:HG13	2.01	0.42
1:C:86:VAL:HG12	4:C:384:HOH:O	2.20	0.42
1:C:127:MET:HG3	1:C:146:TYR:HB2	2.02	0.42
1:A:168:ARG:NH2	1:A:297:PHE:HB3	2.34	0.42
1:C:305:ALA:HB2	1:C:310:THR:OG1	2.19	0.42
1:A:70:LYS:O	1:A:73:ARG:HB3	2.20	0.42
1:B:173:HIS:CE1	1:B:175:LEU:CD2	2.99	0.42
1:B:14:LEU:HD21	1:B:107:MET:CE	2.50	0.41
1:B:194:GLU:HA	1:B:195:ASN:HA	1.72	0.41
1:D:101:LEU:O	1:D:142:THR:HA	2.20	0.41
1:C:119:ARG:HB3	4:C:486:HOH:O	2.19	0.41
1:C:30:SER:HB3	1:C:32:ALA:O	2.20	0.41
1:B:40:GLN:HB3	1:B:41:PRO:HD2	2.03	0.41
1:B:237:HIS:HB3	1:B:242:PHE:CE2	2.55	0.41
1:D:281:THR:HG22	1:D:335:ARG:CG	2.51	0.41
1:D:252:ALA:HB1	1:D:329:HIS:HB2	2.01	0.41
1:A:278:ALA:HB3	1:A:298:PHE:HB2	2.03	0.41
1:B:193:SER:O	1:B:195:ASN:HA	2.21	0.41
1:C:286:LEU:HD13	1:C:331:GLN:NE2	2.36	0.41
1:C:197:ASN:HB3	1:C:204:ALA:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:LEU:HD21	1:C:107:MET:HE1	2.02	0.41
1:B:189:THR:O	1:B:271:HIS:HD2	2.04	0.41
1:D:205:LEU:HD23	1:D:280:MET:CE	2.47	0.40
1:C:184:LEU:HD23	1:C:184:LEU:O	2.20	0.40
1:C:210:LYS:HE3	1:C:329:HIS:CD2	2.55	0.40
1:D:257:ASP:HA	1:D:258:PRO:HD3	1.96	0.40
1:B:278:ALA:HB3	1:B:298:PHE:HB2	2.03	0.40
1:B:176:LEU:N	1:B:176:LEU:HD12	2.36	0.40
1:A:276:TYR:O	1:A:300:PRO:HB3	2.21	0.40
2:X:1001:ASN:HD22	2:X:1001:ASN:C	2.23	0.40
1:B:285:PRO:O	1:B:286:LEU:HD23	2.21	0.40
1:B:74:PHE:HB2	1:B:76:LEU:HD23	2.03	0.40
1:C:225:HIS:CD2	4:C:501:HOH:O	2.74	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	317/370 (86%)	309 (98%)	7 (2%)	1 (0%)	46	50
1	B	334/370 (90%)	325 (97%)	9 (3%)	0	100	100
1	C	321/370 (87%)	308 (96%)	13 (4%)	0	100	100
1	D	322/370 (87%)	311 (97%)	10 (3%)	1 (0%)	46	50
2	X	5/7 (71%)	5 (100%)	0	0	100	100
3	Y	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	1306/1496 (87%)	1264 (97%)	40 (3%)	2 (0%)	52	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	322	GLU
1	D	235	ALA

5.3.2 Protein sidechains ⓘ

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	254/302 (84%)	246 (97%)	8 (3%)	47	59
1	B	270/302 (89%)	249 (92%)	21 (8%)	16	15
1	C	255/302 (84%)	235 (92%)	20 (8%)	16	15
1	D	246/302 (82%)	231 (94%)	15 (6%)	23	26
2	X	5/5 (100%)	3 (60%)	2 (40%)	0	0
3	Y	6/6 (100%)	3 (50%)	3 (50%)	0	0
All	All	1036/1219 (85%)	967 (93%)	69 (7%)	20	21

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	PHE
1	A	83	GLN
1	A	120	LEU
1	A	127	MET
1	A	184	LEU
1	A	187	THR
1	A	189	THR
1	A	240	LEU
1	B	26	ASP
1	B	29	LYS
1	B	70	LYS
1	B	71	LEU
1	B	76	LEU
1	B	103	LEU
1	B	120	LEU
1	B	152	ARG
1	B	157	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	175	LEU
1	B	187	THR
1	B	203	ILE
1	B	209	LEU
1	B	215	ASN
1	B	238	ASP
1	B	240	LEU
1	B	261	PHE
1	B	265	VAL
1	B	280	MET
1	B	306	GLN
1	B	353	LEU
1	C	50	SER
1	C	71	LEU
1	C	82	SER
1	C	103	LEU
1	C	120	LEU
1	C	157	VAL
1	C	175	LEU
1	C	179	SER
1	C	187	THR
1	C	205	LEU
1	C	223	LYS
1	C	225	HIS
1	C	238	ASP
1	C	243	TRP
1	C	270	VAL
1	C	284	ASP
1	C	286	LEU
1	C	287	VAL
1	C	318	VAL
1	C	322	GLU
1	D	26	ASP
1	D	29	LYS
1	D	86	VAL
1	D	103	LEU
1	D	119	ARG
1	D	120	LEU
1	D	128	THR
1	D	157	VAL
1	D	187	THR
1	D	197	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	205	LEU
1	D	270	VAL
1	D	275	LEU
1	D	280	MET
1	D	281	THR
2	X	1001	ASN
2	X	1004	CYS
3	Y	1018	GLU
3	Y	1019	VAL
3	Y	1025	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	166	GLN
1	B	132	GLN
1	B	173	HIS
1	B	185	HIS
1	B	215	ASN
1	B	271	HIS
1	B	321	HIS
1	B	331	GLN
1	C	225	HIS
1	C	331	GLN
1	D	166	GLN
1	D	197	ASN
1	D	331	GLN

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 [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, 95th 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	327/370 (88%)	0.67	22 (6%) 21 20	48, 74, 103, 107	0
1	B	342/370 (92%)	0.66	34 (9%) 9 8	48, 68, 92, 106	0
1	C	331/370 (89%)	0.53	16 (4%) 34 34	51, 68, 97, 109	0
1	D	330/370 (89%)	0.63	21 (6%) 23 22	52, 75, 97, 118	0
2	X	7/7 (100%)	1.71	2 (28%) 1 1	93, 93, 100, 102	0
3	Y	9/9 (100%)	0.48	0 100 100	84, 86, 88, 88	0
All	All	1346/1496 (89%)	0.63	95 (7%) 19 18	48, 71, 99, 118	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	212	PHE	5.4
1	A	181	VAL	5.3
1	C	196	PRO	4.9
1	C	305	ALA	4.4
1	D	215	ASN	4.2
1	A	215	ASN	4.1
1	D	213	GLY	4.1
1	B	182	LEU	4.0
2	X	1000	SER	3.9
1	C	184	LEU	3.9
1	C	192	ALA	3.9
1	C	273	PRO	3.9
1	A	345	PRO	3.6
1	C	234	LYS	3.6
1	B	351	THR	3.5
1	C	189	THR	3.5
1	B	251	ARG	3.4
1	C	188	GLU	3.3
1	D	323	VAL	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	92	VAL	3.2
1	B	349	TYR	3.2
1	B	181	VAL	3.1
1	D	214	GLU	3.0
1	A	189	THR	3.0
1	B	289	GLU	3.0
1	B	28	LEU	2.9
1	B	346	GLU	2.9
1	C	187	THR	2.8
1	B	354	GLY	2.8
1	D	25	GLY	2.8
1	B	156	ILE	2.7
1	A	198	VAL	2.7
1	D	69	ASP	2.7
1	C	236	GLN	2.7
1	C	193	SER	2.7
1	A	182	LEU	2.6
1	D	31	GLU	2.6
1	C	211	GLY	2.6
1	D	179	SER	2.6
1	B	123	PHE	2.6
1	B	194	GLU	2.6
1	A	89	THR	2.6
1	A	213	GLY	2.6
1	B	195	ASN	2.5
2	X	1004	CYS	2.5
1	D	196	PRO	2.5
1	B	25	GLY	2.5
1	D	21	ALA	2.5
1	A	91	CYS	2.5
1	D	307	ALA	2.5
1	B	348	LEU	2.5
1	B	323	VAL	2.5
1	B	305	ALA	2.4
1	D	72	ASN	2.4
1	B	261	PHE	2.4
1	B	23	PHE	2.4
1	A	173	HIS	2.4
1	D	210	LYS	2.4
1	A	179	SER	2.4
1	A	76	LEU	2.4
1	D	324	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	285	PRO	2.3
1	D	24	ALA	2.3
1	B	149	ILE	2.3
1	B	91	CYS	2.3
1	B	294	TYR	2.3
1	B	120	LEU	2.3
1	B	262	TYR	2.3
1	D	23	PHE	2.3
1	C	215	ASN	2.3
1	A	346	GLU	2.3
1	B	32	ALA	2.2
1	B	122	ILE	2.2
1	A	284	ASP	2.2
1	A	186	GLU	2.2
1	A	26	ASP	2.2
1	D	187	THR	2.2
1	A	269	ALA	2.2
1	D	255	ILE	2.1
1	A	250	GLY	2.1
1	B	154	PHE	2.1
1	C	272	VAL	2.1
1	A	11	THR	2.1
1	D	310	THR	2.1
1	C	346	GLU	2.1
1	B	151	PRO	2.1
1	B	199	THR	2.1
1	B	177	ASN	2.1
1	A	190	LEU	2.0
1	B	36	VAL	2.0
1	B	10	THR	2.0
1	B	89	THR	2.0
1	D	10	THR	2.0
1	A	286	LEU	2.0
1	C	173	HIS	2.0

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 [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.