Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:33 PM GMT

PDB ID	:	4FCY
Title	:	Crystal structure of the bacteriophage Mu transpososome
Authors	:	Montano, S.P.; Pigli, Y.Z.; Rice, P.A.
Deposited on	:	2012-05-25
Resolution	:	3.71 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 (1)) were used in the production of this report:

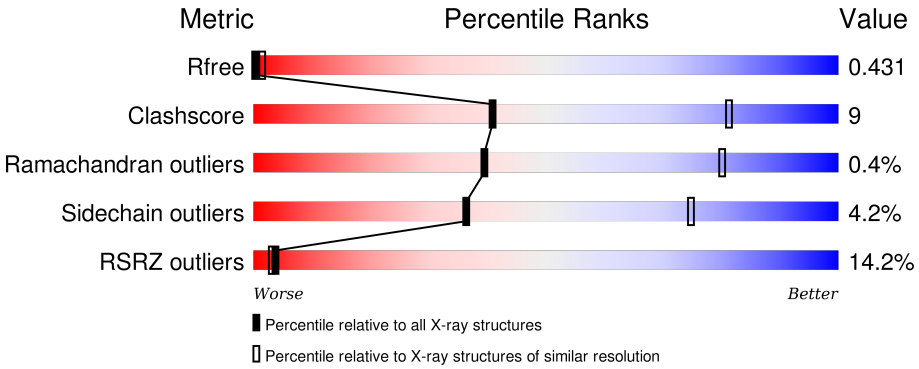
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.71 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}	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)

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.

Mol	Chain	Length	Quality of chain
1	A	529	20% 61% 21% • 16%
1	B	529	7% 69% 19% • 10%
2	C	68	6% 53% 44% •
3	E	13	23% 62% 31% 8%
4	D	49	45% 45% 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10056 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 Transposase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3587	2278	640	651	18			
1	B	476	Total	C	N	O	S	0	0	0
			3810	2423	680	689	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	521	LEU	MET	engineered mutation	UNP P07636
A	525	LEU	ASN	engineered mutation	UNP P07636
B	521	LEU	MET	engineered mutation	UNP P07636
B	525	LEU	ASN	engineered mutation	UNP P07636

- Molecule 2 is a DNA chain called DNA (68-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	68	Total	C	N	O	P	0	0	0
			1384	665	226	426	67			

- Molecule 3 is a DNA chain called DNA (13-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	13	Total	C	N	O	P	0	0	0
			263	125	52	73	13			

- Molecule 4 is a DNA chain called DNA (49-MER).

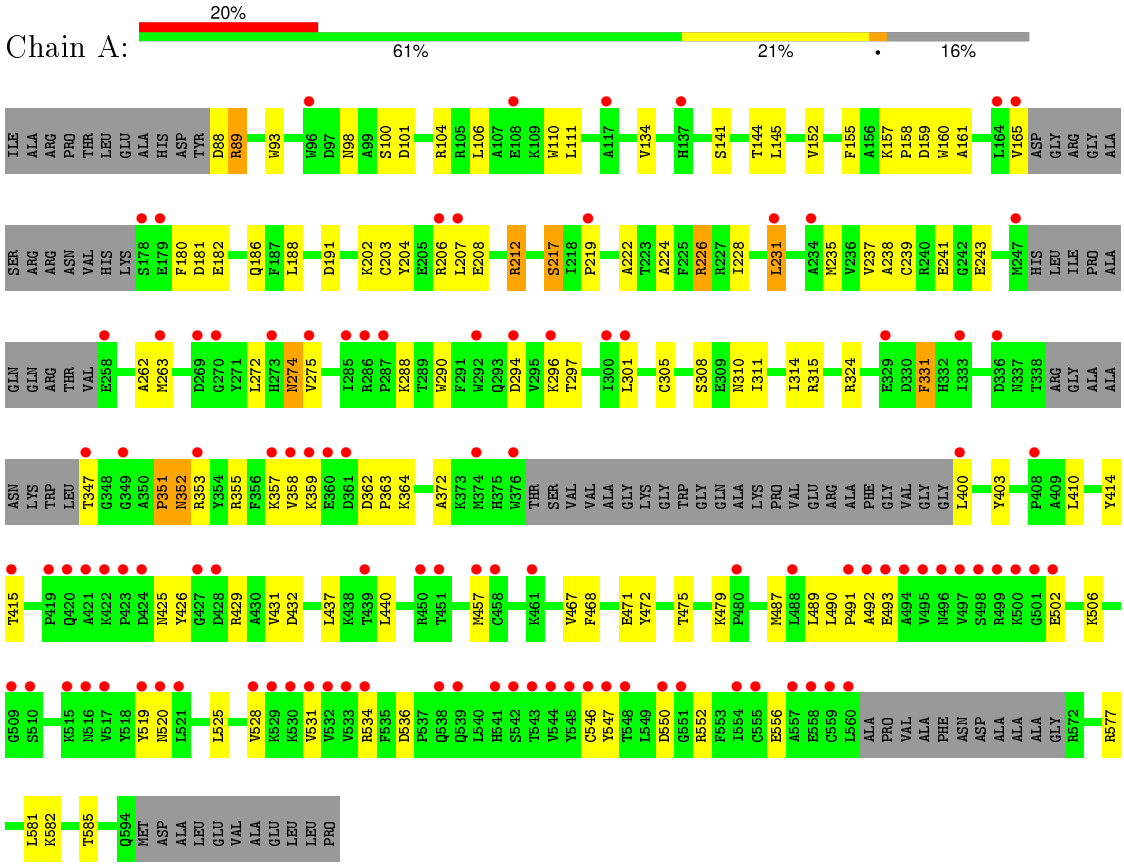
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	49	Total	C	N	O	P	0	0	0
			1012	479	208	277	48			

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.

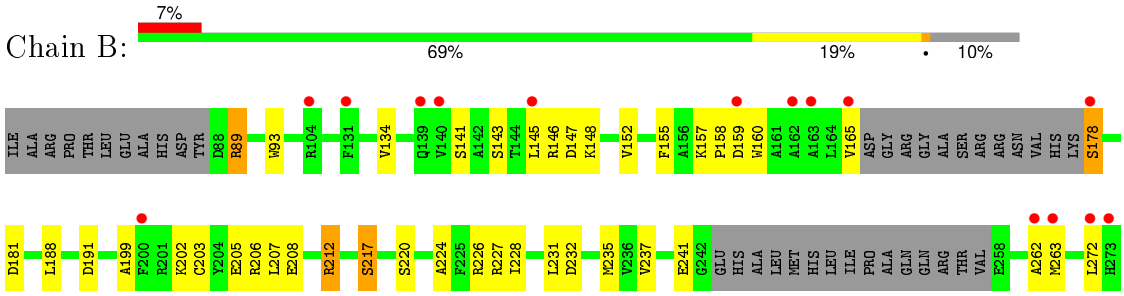
- Molecule 1: Transposase

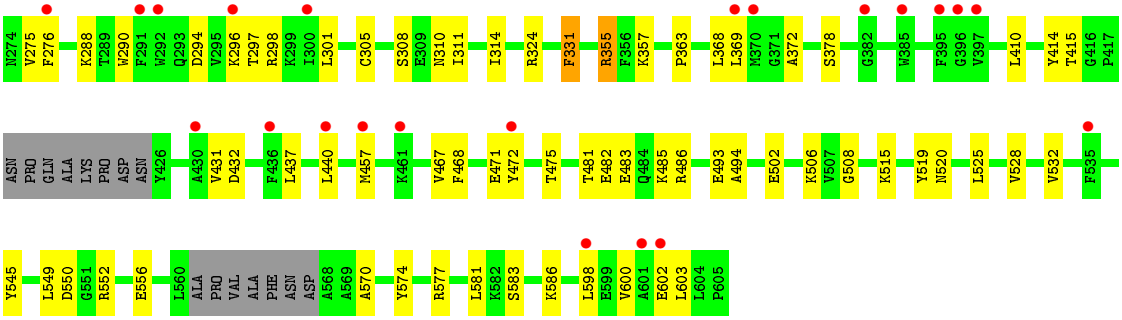
Chain A:



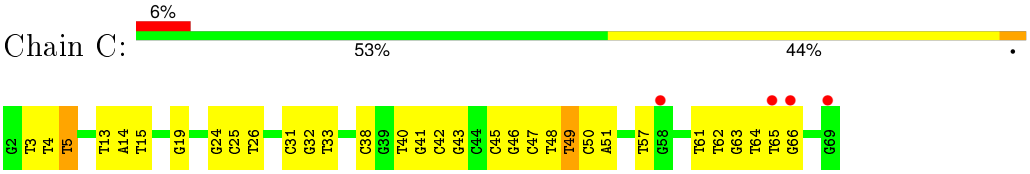
- Molecule 1: Transposase

Chain B:



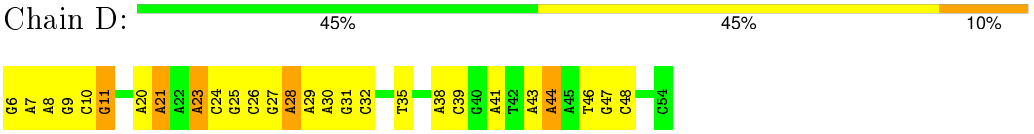


- Molecule 2: DNA (68-MER)



- Molecule 3: DNA (13-MER)

- Molecule 4: DNA (49-MER)



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	196.14Å 196.14Å 349.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.03 – 3.71 49.03 – 3.71	Depositor EDS
% Data completeness (in resolution range)	47.0 (49.03-3.71) 46.1 (49.03-3.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_847)	Depositor
R, R_{free}	0.393 , 0.437 0.382 , 0.431	Depositor DCC
R_{free} test set	859 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	144.3	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 174.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 18803 reflections	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	10056	wwPDB-VP
Average B, all atoms (Å^2)	294.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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, 0.375 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	0.33	0/3667	0.57	0/4945
1	B	0.32	0/3895	0.56	0/5255
2	C	0.69	0/1543	1.46	14/2379 (0.6%)
3	E	0.59	0/295	1.26	2/451 (0.4%)
4	D	0.62	0/1141	1.38	13/1757 (0.7%)
All	All	0.44	0/10541	0.92	29/14787 (0.2%)

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 (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	24	DC	O4'-C1'-N1	8.56	114.00	108.00
2	C	40	DT	O4'-C1'-N1	6.90	112.83	108.00
2	C	41	DG	O4'-C1'-N9	6.86	112.81	108.00
2	C	5	DT	O4'-C1'-N1	6.82	112.77	108.00
2	C	26	DT	O4'-C1'-N1	6.57	112.60	108.00
4	D	46	DT	O4'-C1'-N1	6.46	112.52	108.00
2	C	61	DT	N3-C4-O4	6.13	123.58	119.90
2	C	38	DC	O4'-C1'-N1	6.08	112.26	108.00
4	D	46	DT	C3'-C2'-C1'	-6.06	95.23	102.50
2	C	49	DT	O4'-C1'-N1	6.02	112.22	108.00
4	D	44	DA	O4'-C1'-N9	5.94	112.16	108.00
4	D	6	DG	O4'-C1'-N9	5.94	112.16	108.00
2	C	40	DT	O4'-C1'-C2'	-5.87	101.21	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	48	DT	O4'-C1'-N1	5.82	112.08	108.00
2	C	4	DT	O4'-C1'-N1	5.68	111.98	108.00
2	C	41	DG	C1'-O4'-C4'	-5.49	104.61	110.10
2	C	57	DT	N3-C4-O4	5.44	123.17	119.90
4	D	47	DG	O4'-C1'-N9	5.39	111.77	108.00
4	D	23	DA	C3'-C2'-C1'	-5.35	96.08	102.50
4	D	11	DG	O4'-C1'-N9	5.33	111.73	108.00
4	D	32	DC	O4'-C1'-N1	5.28	111.70	108.00
4	D	35	DT	C5-C4-O4	-5.22	121.25	124.90
4	D	21	DA	O4'-C1'-N9	5.21	111.65	108.00
4	D	46	DT	C1'-O4'-C4'	-5.20	104.90	110.10
3	E	7	DA	O4'-C1'-N9	5.17	111.62	108.00
4	D	28	DA	C3'-C2'-C1'	-5.09	96.39	102.50
2	C	3	DT	O4'-C1'-N1	5.08	111.55	108.00
3	E	9	DA	O4'-C1'-N9	5.07	111.55	108.00
2	C	26	DT	O4'-C1'-C2'	-5.00	101.90	105.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	351	PRO	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	3587	0	3530	77	0
1	B	3810	0	3765	66	0
2	C	1384	0	779	19	0
3	E	263	0	145	3	0
4	D	1012	0	547	16	0
All	All	10056	0	8766	162	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 9.

All (162) 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:489:LEU:HD13	1:A:536:ASP:HB2	1.58	0.83
1:A:111:LEU:HD22	1:B:369:LEU:HD23	1.61	0.80
1:A:144:THR:OG1	4:D:25:DG:OP2	1.99	0.79
1:A:315:ARG:HH22	1:A:534:ARG:HH12	1.27	0.78
1:A:311:ILE:HD13	1:A:363:PRO:HG2	1.65	0.77
1:A:111:LEU:HD23	1:B:368:LEU:HG	1.69	0.73
4:D:27:DG:HO3'	4:D:28:DA:HO5'	1.31	0.73
1:A:315:ARG:NH2	1:A:534:ARG:HH12	1.87	0.71
1:B:272:LEU:HD13	1:B:288:LYS:HE3	1.73	0.70
1:A:272:LEU:HD13	1:A:288:LYS:HE3	1.73	0.70
1:B:600:VAL:HA	1:B:603:LEU:HD23	1.74	0.69
1:A:237:VAL:O	1:A:241:GLU:N	2.27	0.66
1:B:152:VAL:O	1:B:160:TRP:NE1	2.30	0.65
1:A:152:VAL:O	1:A:160:TRP:NE1	2.30	0.64
1:A:351:PRO:HB3	1:A:352:ASN:HB3	1.80	0.64
1:B:355:ARG:HE	1:B:508:GLY:HA3	1.62	0.64
1:A:101:ASP:OD2	1:A:104:ARG:NH2	2.31	0.63
1:B:220:SER:N	2:C:19:DG:OP2	2.33	0.62
1:B:357:LYS:HD2	1:B:493:GLU:HG3	1.81	0.61
1:A:212:ARG:HG2	1:A:212:ARG:HH11	1.65	0.61
1:A:581:LEU:O	1:A:585:THR:HG23	2.01	0.61
1:A:487:MET:SD	1:A:547:TYR:OH	2.59	0.60
1:B:212:ARG:HH11	1:B:212:ARG:HG2	1.65	0.59
1:A:353:ARG:HH21	1:A:490:LEU:HD13	1.66	0.59
1:A:274:ASN:HB3	1:A:414:TYR:CE1	2.37	0.59
1:B:297:THR:HG21	1:B:468:PHE:HA	1.86	0.58
1:B:178:SER:OG	1:B:227:ARG:NH1	2.36	0.58
1:A:400:LEU:HA	1:A:403:TYR:HD2	1.69	0.57
1:B:486:ARG:HD3	1:B:545:TYR:CD2	2.39	0.57
1:A:297:THR:HG21	1:A:468:PHE:HA	1.86	0.56
1:A:410:LEU:HD22	1:A:431:VAL:HG21	1.86	0.56
2:C:33:DT:H3	4:D:23:DA:H61	1.53	0.56
1:B:147:ASP:OD2	4:D:48:DC:N4	2.40	0.54
1:B:220:SER:HG	2:C:19:DG:H8	1.55	0.54
1:B:472:TYR:O	1:B:475:THR:HG22	2.08	0.54
1:B:146:ARG:HH11	2:C:5:DT:H71	1.74	0.54
1:A:224:ALA:O	1:A:228:ILE:HG12	2.09	0.53
2:C:64:DT:O4	3:E:6:DA:N6	2.42	0.53
1:A:274:ASN:HB3	1:A:414:TYR:HE1	1.73	0.53
1:A:301:LEU:O	1:A:324:ARG:NH1	2.42	0.53
2:C:49:DT:H3	4:D:7:DA:H61	1.54	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ASP:OD2	1:B:217:SER:N	2.39	0.53
1:A:582:LYS:O	1:A:585:THR:OG1	2.23	0.52
1:A:358:VAL:HG22	1:A:492:ALA:HA	1.90	0.52
1:B:301:LEU:O	1:B:324:ARG:NH1	2.42	0.52
1:B:532:VAL:HG23	1:B:549:LEU:HD23	1.91	0.52
1:A:237:VAL:HG13	1:A:243:GLU:H	1.75	0.52
1:A:161:ALA:HB2	1:B:369:LEU:HD22	1.91	0.51
1:A:89:ARG:HB3	1:A:93:TRP:CD1	2.45	0.51
1:A:415:THR:HG22	1:A:426:TYR:CZ	2.45	0.51
1:B:506:LYS:HD3	1:B:515:LYS:HG3	1.92	0.51
1:A:155:PHE:O	1:A:160:TRP:NE1	2.44	0.51
1:A:550:ASP:OD2	1:A:552:ARG:NH1	2.44	0.50
1:A:311:ILE:HD11	1:A:347:THR:HA	1.92	0.50
1:B:199:ALA:HB3	1:B:202:LYS:HG2	1.93	0.50
1:A:275:VAL:HG22	1:A:414:TYR:HB2	1.93	0.50
1:A:296:LYS:HE2	1:A:457:MET:SD	2.53	0.49
4:D:38:DA:H2"	4:D:39:DC:C6	2.46	0.49
1:B:577:ARG:O	1:B:581:LEU:HG	2.13	0.49
1:B:288:LYS:HD3	1:B:308:SER:HA	1.95	0.49
1:A:357:LYS:HD2	1:A:493:GLU:HG3	1.94	0.49
1:A:93:TRP:O	1:B:483:GLU:HG2	2.12	0.49
1:A:288:LYS:HD3	1:A:308:SER:HA	1.95	0.49
1:B:89:ARG:HB3	1:B:93:TRP:CD1	2.47	0.49
2:C:45:DC:H2"	2:C:46:DG:C8	2.47	0.49
1:B:296:LYS:HE2	1:B:457:MET:SD	2.52	0.49
1:A:181:ASP:OD2	1:A:217:SER:N	2.42	0.48
1:A:577:ARG:O	1:A:581:LEU:HG	2.12	0.48
1:A:331:PHE:HB3	1:A:372:ALA:HA	1.95	0.48
1:A:355:ARG:HB3	1:A:506:LYS:O	2.14	0.48
1:B:155:PHE:O	1:B:160:TRP:NE1	2.44	0.48
2:C:24:DG:H4'	2:C:25:DC:OP1	2.14	0.47
1:B:410:LEU:HD22	1:B:431:VAL:HG21	1.96	0.47
1:B:331:PHE:HB3	1:B:372:ALA:HA	1.95	0.47
1:A:520:ASN:ND2	1:A:556:GLU:O	2.46	0.47
1:B:188:LEU:HB2	1:B:207:LEU:HD22	1.96	0.47
1:A:202:LYS:O	1:A:206:ARG:HG3	2.14	0.47
1:A:359:LYS:HG2	1:A:491:PRO:HB2	1.96	0.47
2:C:50:DC:H2"	2:C:51:DA:H5'	1.97	0.47
1:A:222:ALA:O	1:A:226:ARG:HB2	2.15	0.47
1:A:235:MET:O	1:A:238:ALA:HB3	2.15	0.47
3:E:9:DA:H2"	3:E:10:DA:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:20:DA:H2"	4:D:21:DA:C8	2.49	0.47
1:A:161:ALA:CB	1:B:369:LEU:HD22	2.45	0.46
1:B:89:ARG:NH1	1:B:89:ARG:HB2	2.30	0.46
2:C:62:DT:H2"	2:C:63:DG:C8	2.51	0.46
1:B:237:VAL:O	1:B:241:GLU:HB2	2.16	0.46
1:B:275:VAL:HG22	1:B:414:TYR:HA	1.97	0.46
1:A:188:LEU:HB2	1:A:207:LEU:HD22	1.98	0.46
1:B:311:ILE:HG21	1:B:363:PRO:HG2	1.98	0.46
1:A:351:PRO:HA	1:A:357:LYS:HG3	1.98	0.46
1:B:570:ALA:O	1:B:574:TYR:HB2	2.15	0.45
1:B:355:ARG:NE	1:B:508:GLY:HA3	2.27	0.45
1:B:482:GLU:OE2	1:B:485:LYS:NZ	2.44	0.45
1:A:180:PHE:CE2	1:A:219:PRO:HB3	2.51	0.45
1:A:359:LYS:HB2	1:A:491:PRO:O	2.16	0.45
2:C:65:DT:H2"	2:C:66:DG:C8	2.51	0.45
1:B:237:VAL:O	1:B:241:GLU:N	2.50	0.45
1:B:224:ALA:O	1:B:228:ILE:HG12	2.17	0.44
4:D:43:DA:H2"	4:D:44:DA:C8	2.52	0.44
1:A:98:ASN:HA	1:B:552:ARG:HG2	1.99	0.44
1:A:212:ARG:HH11	1:A:212:ARG:CG	2.29	0.44
4:D:29:DA:H2"	4:D:30:DA:C8	2.52	0.44
1:A:262:ALA:O	1:A:263:MET:HB2	2.18	0.44
1:A:88:ASP:HA	1:A:89:ARG:NH2	2.32	0.44
1:B:148:LYS:O	1:B:152:VAL:HG22	2.18	0.44
1:B:305:CYS:HB3	1:B:437:LEU:HD21	2.00	0.44
2:C:13:DT:H2"	2:C:14:DA:C8	2.52	0.44
1:B:520:ASN:ND2	1:B:556:GLU:O	2.46	0.44
1:B:494:ALA:HB2	1:B:549:LEU:HD21	1.98	0.44
2:C:15:DT:H3	4:D:41:DA:H61	1.65	0.43
1:A:100:SER:HA	1:B:550:ASP:O	2.18	0.43
1:A:502:GLU:HG2	1:A:519:TYR:CD1	2.53	0.43
1:A:134:VAL:HG11	1:A:145:LEU:HD22	2.01	0.43
1:A:297:THR:HB	1:A:467:VAL:HG23	2.00	0.43
1:B:262:ALA:O	1:B:263:MET:HB2	2.18	0.43
1:B:297:THR:HB	1:B:467:VAL:HG23	2.00	0.43
3:E:8:DC:H2"	3:E:9:DA:C8	2.53	0.43
1:B:134:VAL:HG11	1:B:145:LEU:HD22	2.01	0.43
1:B:502:GLU:HG2	1:B:519:TYR:CD1	2.54	0.43
1:A:362:ASP:OD1	1:A:364:LYS:HB2	2.18	0.43
1:A:93:TRP:CD1	1:B:481:THR:HG21	2.53	0.43
1:A:425:ASN:HB3	1:A:429:ARG:NE	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:TYR:O	1:A:475:THR:HG22	2.17	0.43
4:D:10:DC:H2"	4:D:11:DG:C8	2.54	0.43
1:A:305:CYS:HB3	1:A:437:LEU:HD21	2.01	0.43
4:D:26:DC:H2"	4:D:27:DG:H5"	2.01	0.42
2:C:64:DT:H2"	2:C:65:DT:C6	2.54	0.42
1:B:202:LYS:HG3	1:B:203:CYS:N	2.34	0.42
4:D:8:DA:H2"	4:D:9:DG:C8	2.54	0.42
1:B:212:ARG:HH11	1:B:212:ARG:CG	2.30	0.42
2:C:32:DG:H2"	2:C:33:DT:C6	2.54	0.42
1:A:228:ILE:HA	1:A:231:LEU:HG	2.02	0.42
1:B:598:LEU:O	1:B:602:GLU:HG2	2.18	0.42
1:A:479:LYS:HA	1:A:479:LYS:HD3	1.90	0.42
2:C:31:DC:H2"	2:C:32:DG:C8	2.54	0.42
1:A:182:GLU:O	1:A:186:GLN:HG3	2.20	0.42
1:A:274:ASN:ND2	1:A:274:ASN:O	2.41	0.42
1:A:531:VAL:HG21	1:A:546:CYS:HB3	2.02	0.42
1:A:351:PRO:CB	1:A:352:ASN:HB3	2.49	0.41
1:A:294:ASP:HB2	1:A:301:LEU:HD11	2.01	0.41
1:B:276:PHE:CE2	1:B:415:THR:HG21	2.55	0.41
1:A:296:LYS:NZ	1:A:471:GLU:OE1	2.53	0.41
1:B:296:LYS:NZ	1:B:471:GLU:OE1	2.53	0.41
1:B:232:ASP:HB3	1:B:235:MET:HG2	2.02	0.41
4:D:30:DA:H2"	4:D:31:DG:C8	2.56	0.41
1:A:191:ASP:HB3	1:A:203:CYS:SG	2.60	0.41
1:A:204:TYR:O	1:A:208:GLU:HG3	2.20	0.41
1:B:290:TRP:CD2	1:B:314:ILE:HG12	2.56	0.41
1:B:583:SER:HA	1:B:586:LYS:HD2	2.02	0.41
1:B:143:SER:HB3	4:D:48:DC:C5	2.55	0.41
1:B:294:ASP:HB2	1:B:301:LEU:HD11	2.01	0.41
2:C:46:DG:H2"	2:C:47:DC:C6	2.56	0.41
1:B:157:LYS:N	1:B:158:PRO:HD2	2.36	0.41
1:B:205:GLU:O	1:B:208:GLU:HB2	2.21	0.40
1:A:290:TRP:CD2	1:A:314:ILE:HG12	2.56	0.40
1:A:157:LYS:N	1:A:158:PRO:HD2	2.36	0.40
1:B:298:ARG:HA	1:B:298:ARG:HD3	1.87	0.40
1:A:106:LEU:O	1:A:110:TRP:HD1	2.04	0.40
2:C:49:DT:H3	4:D:7:DA:N6	2.17	0.40
1:B:290:TRP:CG	1:B:314:ILE:HG12	2.57	0.40
2:C:42:DC:H2"	2:C:43:DG:C8	2.57	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	431/529 (82%)	414 (96%)	15 (4%)	2 (0%)	34 77
1	B	466/529 (88%)	450 (97%)	14 (3%)	2 (0%)	39 80
All	All	897/1058 (85%)	864 (96%)	29 (3%)	4 (0%)	39 80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	352	ASN
1	B	355	ARG
1	A	231	LEU
1	B	231	LEU

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	370/430 (86%)	355 (96%)	15 (4%)	37 75
1	B	387/430 (90%)	370 (96%)	17 (4%)	35 74
All	All	757/860 (88%)	725 (96%)	32 (4%)	36 75

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

Mol	Chain	Res	Type
1	A	89	ARG
1	A	141	SER

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Mol	Chain	Res	Type
1	A	159	ASP
1	A	165	VAL
1	A	212	ARG
1	A	217	SER
1	A	226	ARG
1	A	239	CYS
1	A	274	ASN
1	A	310	ASN
1	A	331	PHE
1	A	432	ASP
1	A	440	LEU
1	A	525	LEU
1	A	528	VAL
1	B	89	ARG
1	B	141	SER
1	B	159	ASP
1	B	165	VAL
1	B	178	SER
1	B	191	ASP
1	B	206	ARG
1	B	212	ARG
1	B	217	SER
1	B	226	ARG
1	B	310	ASN
1	B	331	PHE
1	B	378	SER
1	B	432	ASP
1	B	440	LEU
1	B	525	LEU
1	B	528	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	267	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

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	443/529 (83%)	1.28	105 (23%) 1 1	134, 303, 577, 797	0
1	B	476/529 (89%)	0.37	37 (7%) 16 9	130, 264, 400, 526	0
2	C	68/68 (100%)	0.05	4 (5%) 26 15	200, 257, 409, 476	0
3	E	13/13 (100%)	1.21	3 (23%) 1 1	290, 364, 508, 517	0
4	D	49/49 (100%)	-0.57	0 100 100	201, 257, 336, 350	0
All	All	1049/1188 (88%)	0.70	149 (14%) 4 3	130, 277, 475, 797	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	492	ALA	30.3
1	A	532	VAL	12.8
1	A	542	SER	12.0
1	A	559	CYS	11.0
1	A	358	VAL	10.6
1	A	359	LYS	10.3
1	A	502	GLU	9.0
1	A	496	ASN	8.6
1	A	554	ILE	7.2
1	A	499	ARG	7.1
1	A	560	LEU	7.0
1	A	510	SER	6.8
1	A	457	MET	6.7
1	A	550	ASP	6.7
1	B	162	ALA	6.7
1	A	519	TYR	6.6
1	A	538	GLN	6.4
1	B	602	GLU	6.4
1	A	301	LEU	6.2
1	A	285	ILE	6.1

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Mol	Chain	Res	Type	RSRZ
1	B	397	VAL	6.0
1	A	428	ASP	5.9
1	A	516	ASN	5.9
1	A	546	CYS	5.7
1	B	396	GLY	5.5
1	A	531	VAL	5.3
1	A	545	TYR	5.1
1	A	547	TYR	5.1
1	B	165	VAL	5.0
1	A	495	VAL	5.0
1	A	509	GLY	5.0
1	A	501	GLY	4.9
1	A	539	GLN	4.8
1	A	347	THR	4.8
1	A	555	CYS	4.7
1	A	349	GLY	4.7
1	A	361	ASP	4.7
1	A	517	VAL	4.6
1	A	273	HIS	4.6
1	A	520	ASN	4.6
1	A	424	ASP	4.6
1	A	491	PRO	4.6
1	A	178	SER	4.5
1	A	498	SER	4.5
1	B	601	ALA	4.5
1	A	515	LYS	4.5
1	A	529	LYS	4.5
1	A	287	PRO	4.4
1	A	420	GLN	4.3
1	B	272	LEU	4.2
1	A	415	THR	4.1
1	A	263	MET	4.0
1	A	296	LYS	4.0
1	B	262	ALA	4.0
1	A	541	HIS	3.9
1	A	357	LYS	3.9
1	A	493	GLU	3.8
1	A	421	ALA	3.8
1	A	497	VAL	3.8
1	B	296	LYS	3.8
2	C	69	DG	3.7
1	B	178	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	270	GLY	3.7
1	A	275	VAL	3.6
3	E	3	DG	3.6
1	A	360	GLU	3.6
1	B	436	PHE	3.5
1	B	276	PHE	3.4
1	A	530	LYS	3.4
1	A	451	THR	3.4
1	B	535	PHE	3.3
1	A	108	GLU	3.3
1	A	376	TRP	3.3
1	A	427	GLY	3.3
1	A	423	PRO	3.3
1	A	137	HIS	3.2
2	C	66	DG	3.2
1	A	500	LYS	3.2
1	A	548	THR	3.2
3	E	10	DA	3.1
1	A	533	VAL	3.1
1	A	179	GLU	3.1
1	A	336	ASP	3.1
1	A	408	PRO	3.1
1	B	200	PHE	3.0
1	A	286	ARG	3.0
1	B	430	ALA	3.0
1	A	558	GLU	2.9
1	B	159	ASP	2.9
1	A	292	TRP	2.9
1	A	300	ILE	2.9
3	E	2	DC	2.9
1	A	528	VAL	2.8
1	A	206	ARG	2.8
1	A	374	MET	2.8
1	B	382	GLY	2.8
1	B	385	TRP	2.7
1	A	488	LEU	2.7
1	A	557	ALA	2.7
1	A	231	LEU	2.7
1	A	461	LYS	2.7
1	B	395	PHE	2.7
1	A	294	ASP	2.7
2	C	58	DG	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	104	ARG	2.6
1	A	450	ARG	2.6
1	B	461	LYS	2.6
1	A	219	PRO	2.6
1	B	263	MET	2.6
1	B	292	TRP	2.6
1	A	458	CYS	2.6
1	A	480	PRO	2.6
1	B	300	ILE	2.6
1	B	291	PHE	2.5
1	B	145	LEU	2.5
1	A	544	VAL	2.5
2	C	65	DT	2.4
1	A	247	MET	2.4
1	A	269	ASP	2.4
1	B	140	VAL	2.4
1	B	598	LEU	2.4
1	B	370	MET	2.4
1	B	440	LEU	2.4
1	A	165	VAL	2.3
1	A	551	GLY	2.3
1	A	117	ALA	2.3
1	A	333	ILE	2.3
1	B	139	GLN	2.3
1	A	521	LEU	2.3
1	A	494	ALA	2.2
1	B	273	HIS	2.2
1	A	234	ALA	2.2
1	A	422	LYS	2.2
1	A	419	PRO	2.2
1	B	457	MET	2.2
1	B	472	TYR	2.2
1	A	353	ARG	2.2
1	A	164	LEU	2.2
1	B	369	LEU	2.2
1	A	534	ARG	2.1
1	A	258	GLU	2.1
1	A	329	GLU	2.1
1	A	543	THR	2.1
1	B	163	ALA	2.1
1	A	400	LEU	2.1
1	B	131	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	96	TRP	2.0
1	A	207	LEU	2.0
1	A	439	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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.