Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 10:19 AM EDT

PDB ID	:	4WSE
Title	:	Crystal structure of the Mimivirus polyadenylate synthase
Authors	:	Priet, S.; Lartigue, A.; Claverie, J.M.; Abergel, C.
Deposited on	:	2014-10-27
Resolution	:	2.84 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 (i) 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 (1)) were used in the production of this report:

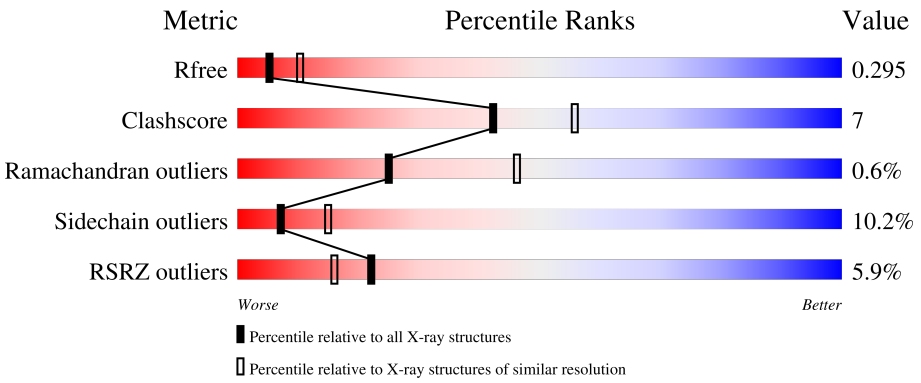
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.84 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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	584	3% 66% 16% • 15%
1	B	584	7% 64% 18% • 15%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8506 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 Putative poly(A) polymerase catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	495	4132	2662	677	780	13	0	1	0
1	B	495	4134	2666	675	780	13	0	0	0

- Molecule 2 is water.

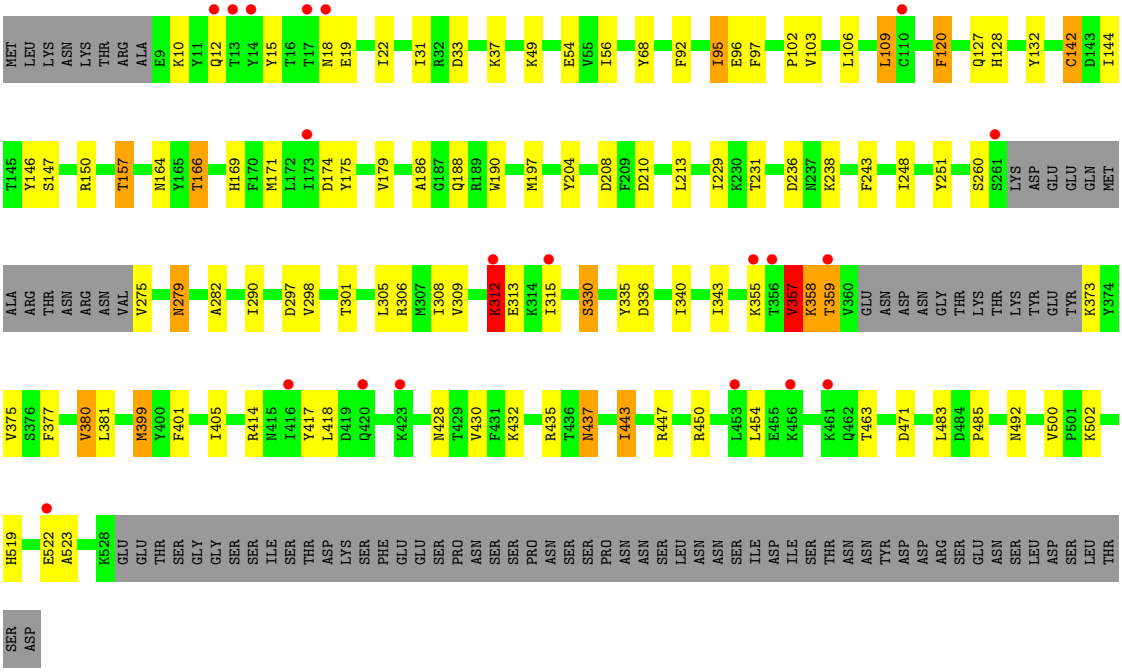
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	122	122	122	0	0
2	B	118	118	118	0	0

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.

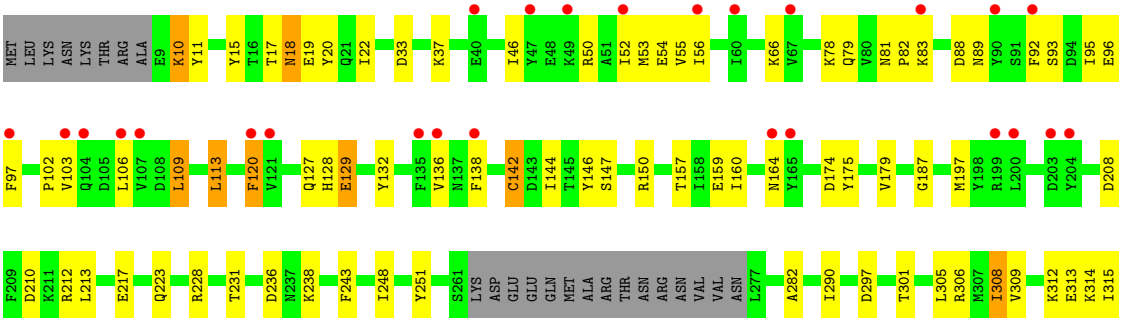
• Molecule 1: Putative poly(A) polymerase catalytic subunit

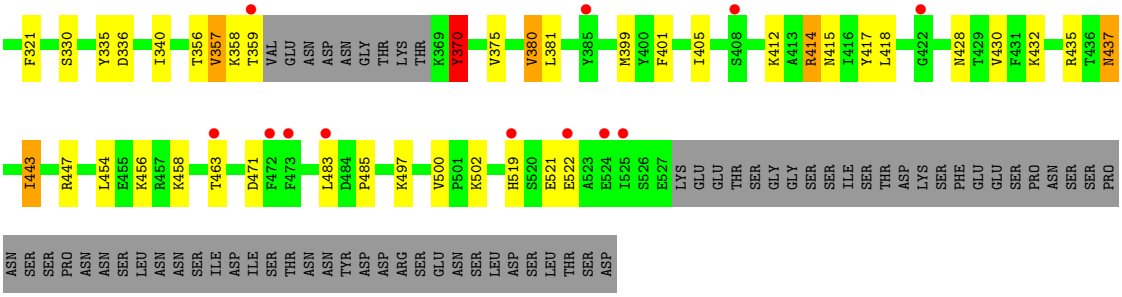
Chain A:



• Molecule 1: Putative poly(A) polymerase catalytic subunit

Chain B:




F321
S330
Y335
D336
I340
T356
V357
K358
T359
VAL
GLU
ASN
ASP
ASN
GLY
THR
LYS
THR
K369
Y370
V375
V380
L381
Y385
M399
Y400
F401
I405
S408
K412
A413
R414
N415
I416
Y417
L418
G422
N428
T429
V430
F431
K432
R435
T436
N437
I443
R447
L454
E455
K456
R457
K458
T463
D471
F472
F473
L483
D484
P485
K497
V500
P501
K502
H519
S520
E521
E522
A523
E524
I525
S526
E527
LYS
GLU
GLU
THR
SER
GLY
GLY
SER
SER
ILE
SER
THR
ASP
LYS
SER
PHE
GLU
GLU
SER
PRO
ASN
SER
SER
PRO
ASN
SER
SER
PRO
ASN
ASN
SER
LEU
ASN
ASN
SER
ILE
ASP
ILE
SER
THR
ASN
ASN
TYR
ASP
ASP
ARG
SER
GLU
ASN
SER
LEU
ASP
SER
LEU
THR
SER
ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	200.03Å 69.65Å 97.49Å 90.00° 105.75° 90.00°	Depositor
Resolution (Å)	46.01 – 2.84 46.01 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.01-2.84) 99.3 (46.01-2.84)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 2.86Å)	Xtriage
Refinement program	BUSTER-TNT 2.10.2	Depositor
R, R_{free}	0.227 , 0.268 0.248 , 0.295	Depositor DCC
R_{free} test set	1521 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	70.1	Xtriage
Anisotropy	0.888	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 97.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8506	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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 (i)

5.1 Standard geometry (i)

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	0.52	0/4225	0.80	4/5706 (0.1%)
1	B	0.52	0/4229	0.86	11/5711 (0.2%)
All	All	0.52	0/8454	0.83	15/11417 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	88	ASP	N-CA-C	13.42	147.22	111.00
1	B	89	ASN	N-CA-CB	12.26	132.67	110.60
1	B	10	LYS	N-CA-C	10.57	139.54	111.00
1	A	357	VAL	N-CA-C	9.64	137.03	111.00
1	B	10	LYS	CB-CA-C	-9.42	91.57	110.40
1	A	357	VAL	CB-CA-C	-9.24	93.84	111.40
1	B	89	ASN	N-CA-C	-8.89	87.00	111.00
1	B	128	HIS	N-CA-C	7.62	131.57	111.00
1	B	88	ASP	CB-CA-C	-7.56	95.28	110.40
1	A	358	LYS	N-CA-CB	-7.52	97.06	110.60
1	B	11	TYR	N-CA-CB	-6.86	98.26	110.60
1	B	11	TYR	N-CA-C	6.53	128.63	111.00
1	B	129	GLU	N-CA-CB	6.52	122.33	110.60
1	B	370	TYR	N-CA-C	6.38	128.23	111.00
1	A	358	LYS	C-N-CA	5.92	136.51	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4132	0	4077	63	0
1	B	4134	0	4072	60	0
2	A	122	0	0	3	0
2	B	118	0	0	6	0
All	All	8506	0	8149	113	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 7.

All (113) 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:12:GLN:NE2	1:B:412:LYS:HG3	1.46	1.29
1:B:357:VAL:HA	1:B:370:TYR:O	1.46	1.14
1:A:208:ASP:HB3	1:B:10:LYS:O	1.44	1.14
1:A:12:GLN:HE22	1:B:412:LYS:HG3	0.94	1.08
1:A:358:LYS:HB3	1:A:359:THR:HB	1.48	0.93
1:A:12:GLN:NE2	1:B:412:LYS:CG	2.34	0.89
1:A:208:ASP:CB	1:B:10:LYS:O	2.22	0.87
1:A:357:VAL:HG12	1:A:357:VAL:O	1.79	0.82
1:B:321:PHE:HE1	1:B:522:GLU:HG2	1.45	0.79
1:A:298:VAL:HG22	1:A:343:ILE:HG21	1.67	0.77
1:B:305:LEU:O	1:B:309:VAL:HB	1.87	0.74
1:A:95:ILE:O	1:A:142:CYS:HB2	1.90	0.71
1:A:56:ILE:HG23	1:A:109:LEU:HD11	1.74	0.70
1:A:443:ILE:HG23	1:A:447:ARG:HB3	1.76	0.68
1:A:12:GLN:HE22	1:B:412:LYS:CG	1.89	0.68
1:B:443:ILE:HG23	1:B:447:ARG:HB3	1.75	0.68
1:A:375:VAL:HG23	1:A:380:VAL:HG12	1.74	0.68
1:B:375:VAL:HG23	1:B:380:VAL:HG12	1.74	0.68
1:B:56:ILE:HG23	1:B:109:LEU:HD11	1.77	0.67
1:A:157:THR:HG21	1:A:164:ASN:HB3	1.77	0.67
1:A:492:ASN:H	1:A:523:ALA:HB1	1.62	0.64
1:A:401:PHE:O	1:A:405:ILE:HG12	1.98	0.64
1:A:492:ASN:N	1:A:523:ALA:HB1	2.12	0.63
1:B:401:PHE:O	1:B:405:ILE:HG12	1.99	0.62
1:B:502:LYS:O	1:B:519:HIS:HB2	1.98	0.62
1:A:502:LYS:O	1:A:519:HIS:HB2	1.99	0.62
1:A:166:THR:CG2	1:A:171:MET:CG	2.79	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:PHE:CE1	1:B:522:GLU:HG2	2.32	0.61
1:A:166:THR:HG22	1:A:171:MET:CG	2.31	0.61
1:A:298:VAL:HG22	1:A:343:ILE:HD13	1.82	0.61
1:A:166:THR:CG2	1:A:171:MET:HG3	2.31	0.60
1:B:497:LYS:HG3	2:B:700:HOH:O	2.01	0.59
1:B:50:ARG:HA	1:B:53:MET:HE2	1.85	0.59
1:A:309:VAL:HG21	1:A:315:ILE:HD11	1.85	0.58
1:A:312:LYS:HD2	1:A:312:LYS:H	1.68	0.58
1:B:213:LEU:HD13	1:B:282:ALA:HB2	1.87	0.57
1:A:236:ASP:OD1	1:A:238:LYS:HG2	2.06	0.56
1:A:213:LEU:HD13	1:A:282:ALA:HB2	1.88	0.55
1:A:335:TYR:HB3	1:A:340:ILE:HD11	1.88	0.55
1:B:197:MET:HA	2:B:654:HOH:O	2.07	0.54
1:A:248:ILE:HA	1:A:251:TYR:HB3	1.88	0.54
1:B:236:ASP:OD1	1:B:238:LYS:HG2	2.08	0.54
1:B:248:ILE:HA	1:B:251:TYR:HB3	1.88	0.54
1:A:305:LEU:O	1:A:309:VAL:HB	2.07	0.54
1:A:10:LYS:HB3	1:B:208:ASP:HB3	1.89	0.54
1:A:106:LEU:HD13	1:A:132:TYR:HB3	1.90	0.53
1:A:175:TYR:HB3	1:A:197:MET:HE2	1.91	0.53
1:B:290:ILE:HD12	1:B:375:VAL:HG11	1.91	0.53
1:A:432:LYS:HB3	1:A:435:ARG:HH11	1.73	0.52
1:A:290:ILE:HD12	1:A:375:VAL:HG11	1.92	0.52
1:A:243:PHE:CZ	1:A:297:ASP:HB3	2.45	0.52
1:A:492:ASN:H	1:A:523:ALA:CB	2.22	0.52
1:B:357:VAL:HG23	1:B:370:TYR:HB3	1.91	0.52
1:B:55:VAL:HG11	1:B:113:LEU:HD22	1.92	0.52
1:B:19:GLU:HA	1:B:22:ILE:HD12	1.92	0.52
1:B:243:PHE:CZ	1:B:297:ASP:HB3	2.45	0.51
1:B:175:TYR:HB3	1:B:197:MET:HE2	1.93	0.50
1:A:188:GLN:HG2	2:A:629:HOH:O	2.11	0.50
1:B:228:ARG:CZ	1:B:308:ILE:HG13	2.42	0.50
1:A:357:VAL:O	1:A:357:VAL:CG1	2.45	0.49
1:A:166:THR:HG22	1:A:171:MET:HG3	1.92	0.49
1:A:315:ILE:HD13	1:A:335:TYR:HB2	1.94	0.49
1:B:106:LEU:HD13	1:B:132:TYR:HB3	1.93	0.49
1:A:120:PHE:N	1:A:120:PHE:CD1	2.81	0.49
1:A:56:ILE:HB	1:A:95:ILE:HD11	1.95	0.48
1:A:450:ARG:HD2	1:B:138:PHE:HB3	1.97	0.47
1:A:103:VAL:HG12	2:A:617:HOH:O	2.15	0.47
1:A:19:GLU:HA	1:A:22:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:MET:HG2	2:A:645:HOH:O	2.14	0.47
1:B:217:GLU:HG2	1:B:223:GLN:NE2	2.30	0.47
1:B:197:MET:CA	2:B:654:HOH:O	2.63	0.47
1:A:31:ILE:HG23	1:B:187:GLY:HA2	1.97	0.46
1:A:437:ASN:ND2	1:A:437:ASN:H	2.13	0.46
1:A:103:VAL:HG22	1:A:485:PRO:HB3	1.97	0.46
1:B:314:LYS:HB2	1:B:335:TYR:CE1	2.51	0.46
1:A:298:VAL:HG22	1:A:343:ILE:CG2	2.42	0.46
1:B:97:PHE:CZ	1:B:144:ILE:HG12	2.50	0.46
1:B:414:ARG:HG3	1:B:415:ASN:N	2.30	0.46
1:B:159:GLU:HB2	2:B:716:HOH:O	2.14	0.46
1:B:17:THR:HA	2:B:710:HOH:O	2.15	0.46
1:B:102:PRO:HG3	1:B:146:TYR:HB2	1.98	0.46
1:B:335:TYR:HB2	1:B:340:ILE:HD11	1.98	0.46
1:A:166:THR:CG2	1:A:171:MET:HG2	2.45	0.45
1:B:17:THR:HA	1:B:18:ASN:HA	1.76	0.45
1:A:97:PHE:CZ	1:A:144:ILE:HG12	2.53	0.44
1:B:309:VAL:HG21	1:B:315:ILE:HD11	1.99	0.44
1:A:12:GLN:HE21	1:B:412:LYS:CG	2.25	0.44
1:B:437:ASN:ND2	1:B:437:ASN:H	2.15	0.44
1:B:95:ILE:HB	1:B:142:CYS:HB2	2.00	0.44
1:B:52:ILE:HG23	1:B:113:LEU:HD11	2.00	0.44
1:B:157:THR:HG21	1:B:164:ASN:HB3	1.99	0.44
1:B:103:VAL:HG22	1:B:485:PRO:HB3	2.01	0.43
1:A:229:ILE:HD11	1:A:305:LEU:HD21	2.00	0.43
1:A:102:PRO:HG3	1:A:146:TYR:HB2	2.00	0.43
1:B:78:LYS:HA	1:B:81:ASN:O	2.19	0.42
1:A:417:TYR:HD2	1:A:418:LEU:HD12	1.84	0.42
1:B:78:LYS:HG3	1:B:82:PRO:HA	2.01	0.42
1:B:212:ARG:HB3	1:B:212:ARG:NH1	2.34	0.42
1:B:522:GLU:H	1:B:522:GLU:CD	2.22	0.42
1:A:377:PHE:CE2	1:A:414:ARG:HD3	2.53	0.42
1:A:169:HIS:HE1	1:A:204:TYR:O	2.03	0.42
1:B:432:LYS:HB3	1:B:435:ARG:NH1	2.35	0.42
1:B:335:TYR:CB	1:B:340:ILE:HD11	2.50	0.42
1:A:186:ALA:HA	1:A:190:TRP:CD1	2.55	0.42
1:A:335:TYR:CB	1:A:340:ILE:HD11	2.50	0.41
1:B:417:TYR:HD2	1:B:418:LEU:HD12	1.86	0.41
1:B:20:TYR:HB3	2:B:710:HOH:O	2.19	0.41
1:A:68:TYR:CZ	1:A:96:GLU:HB3	2.55	0.41
1:B:120:PHE:O	1:B:136:VAL:HA	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:ARG:HB3	1:B:212:ARG:HH11	1.86	0.40
1:B:79:GLN:CD	1:B:160:ILE:HG12	2.42	0.40
1:A:49:LYS:HD2	1:A:92:PHE:HA	2.04	0.40
1:A:330:SER:HA	1:A:343:ILE:O	2.21	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	490/584 (84%)	443 (90%)	42 (9%)	5 (1%)	15	31
1	B	489/584 (84%)	446 (91%)	42 (9%)	1 (0%)	47	69
All	All	979/1168 (84%)	889 (91%)	84 (9%)	6 (1%)	25	46

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	ASN
1	A	312	LYS
1	A	359	THR
1	A	15	TYR
1	B	15	TYR
1	A	357	VAL

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	459/542 (85%)	416 (91%)	43 (9%)	8 18
1	B	458/542 (84%)	408 (89%)	50 (11%)	6 13
All	All	917/1084 (85%)	824 (90%)	93 (10%)	7 15

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	33	ASP
1	A	37	LYS
1	A	54	GLU
1	A	95	ILE
1	A	109	LEU
1	A	120	PHE
1	A	127	GLN
1	A	128	HIS
1	A	142	CYS
1	A	147	SER
1	A	150	ARG
1	A	157	THR
1	A	166	THR
1	A	174	ASP
1	A	179	VAL
1	A	210	ASP
1	A	231	THR
1	A	260	SER
1	A	275	VAL
1	A	279	ASN
1	A	301	THR
1	A	306	ARG
1	A	308	ILE
1	A	312	LYS
1	A	313	GLU
1	A	330	SER
1	A	336	ASP
1	A	355	LYS
1	A	373	LYS
1	A	380	VAL
1	A	381	LEU
1	A	399	MET
1	A	428	ASN

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Mol	Chain	Res	Type
1	A	430	VAL
1	A	437	ASN
1	A	443	ILE
1	A	454	LEU
1	A	463	THR
1	A	471	ASP
1	A	483	LEU
1	A	500	VAL
1	A	522	GLU
1	B	18	ASN
1	B	33	ASP
1	B	37	LYS
1	B	46	ILE
1	B	54	GLU
1	B	66	LYS
1	B	83	LYS
1	B	92	PHE
1	B	93	SER
1	B	96	GLU
1	B	109	LEU
1	B	113	LEU
1	B	120	PHE
1	B	127	GLN
1	B	129	GLU
1	B	142	CYS
1	B	147	SER
1	B	150	ARG
1	B	174	ASP
1	B	179	VAL
1	B	210	ASP
1	B	231	THR
1	B	301	THR
1	B	306	ARG
1	B	308	ILE
1	B	312	LYS
1	B	313	GLU
1	B	330	SER
1	B	336	ASP
1	B	356	THR
1	B	357	VAL
1	B	358	LYS
1	B	359	THR

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Mol	Chain	Res	Type
1	B	370	TYR
1	B	380	VAL
1	B	381	LEU
1	B	399	MET
1	B	414	ARG
1	B	428	ASN
1	B	430	VAL
1	B	437	ASN
1	B	443	ILE
1	B	454	LEU
1	B	456	LYS
1	B	458	LYS
1	B	463	THR
1	B	471	ASP
1	B	483	LEU
1	B	500	VAL
1	B	521	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	437	ASN
1	B	223	GLN

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 (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 (i)

6.1 Protein, DNA and RNA chains (i)

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	495/584 (84%)	0.29	20 (4%)	38	30	46, 93, 136, 164	0
1	B	495/584 (84%)	0.46	38 (7%)	13	8	52, 103, 153, 183	5 (1%)
All	All	990/1168 (84%)	0.38	58 (5%)	22	16	46, 99, 142, 183	5 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	52	ILE	5.1
1	B	135	PHE	4.9
1	B	56	ILE	4.9
1	B	67	VAL	4.6
1	B	165	TYR	4.4
1	B	103	VAL	4.1
1	B	104	GLN	3.7
1	A	12	GLN	3.6
1	B	525	ILE	3.5
1	A	461	LYS	3.5
1	B	121	VAL	3.4
1	A	13	THR	3.4
1	B	199	ARG	3.4
1	A	312	LYS	3.4
1	B	49	LYS	3.2
1	B	47	TYR	3.2
1	B	90	TYR	3.2
1	B	106	LEU	3.1
1	B	136	VAL	3.1
1	B	359	THR	3.1
1	A	522	GLU	3.1
1	B	107	VAL	3.0
1	B	138	PHE	3.0
1	A	423	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	463	THR	2.8
1	B	204	TYR	2.8
1	A	420	GLN	2.8
1	A	261	SER	2.8
1	A	17	THR	2.8
1	B	483	LEU	2.8
1	B	422	GLY	2.7
1	A	18	ASN	2.7
1	B	385	TYR	2.6
1	A	356	THR	2.5
1	B	120	PHE	2.5
1	B	524	GLU	2.5
1	A	315	ILE	2.5
1	A	110	CYS	2.5
1	A	453	LEU	2.5
1	B	519	HIS	2.4
1	B	97	PHE	2.4
1	A	456	LYS	2.3
1	B	203	ASP	2.3
1	B	83	LYS	2.3
1	A	14	TYR	2.3
1	B	40	GLU	2.2
1	B	408	SER	2.2
1	A	355	LYS	2.2
1	B	92	PHE	2.1
1	B	473	PHE	2.1
1	B	60	ILE	2.1
1	B	200	LEU	2.1
1	B	472	PHE	2.1
1	A	173	ILE	2.0
1	A	359	THR	2.0
1	B	522	GLU	2.0
1	A	416	ILE	2.0
1	B	164	ASN	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 monosaccharides 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.