Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:13 PM GMT

PDB ID	:	3TAM
Title	:	Crystal structure of HIV-1 reverse transcriptase (K103N mutant) in complex with inhibitor M06
Authors	:	Yan, Y.
Deposited on	:	2011-08-04
Resolution	:	2.51 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:

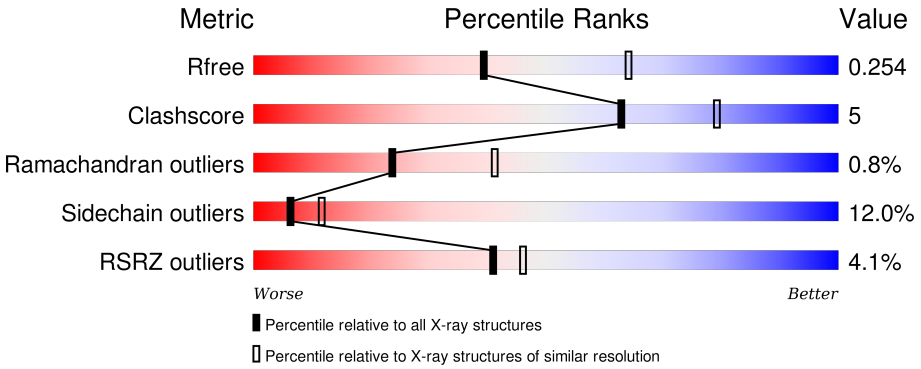
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.51 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	563	3% 76% 20%
2	B	443	5% 71% 17% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8227 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	0	0
			4503	2910	753	832	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	EXPRESSION TAG	UNP P04585
A	-1	ASN	-	EXPRESSION TAG	UNP P04585
A	0	SER	-	EXPRESSION TAG	UNP P04585
A	1	PRO	-	EXPRESSION TAG	UNP P04585
A	2	ILE	-	EXPRESSION TAG	UNP P04585
A	103	ASN	LYS	ENGINEERED MUTATION	UNP P04585

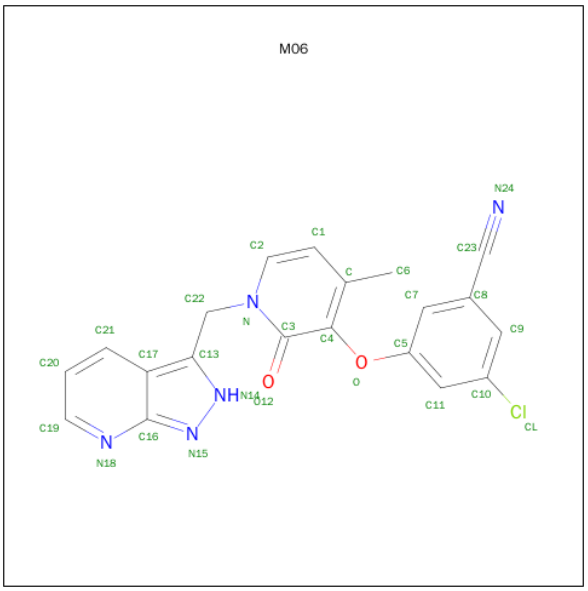
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	403	Total	C	N	O	S	0	0	0
			3334	2170	552	606	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	MET	-	EXPRESSION TAG	UNP P04585
B	-1	ASN	-	EXPRESSION TAG	UNP P04585
B	0	SER	-	EXPRESSION TAG	UNP P04585
B	103	ASN	LYS	ENGINEERED MUTATION	UNP P04585

- Molecule 3 is 3-CHLORO-5-{[4-METHYL-2-OXO-1-(2H-PYRAZOLO[3,4-B]PYRIDIN-3-YLMETHYL)-1,2-DIHYDROPYRIDIN-3-YL]OXY}BENZONITRILE (three-letter code: M06) (formula: $C_{20}H_{14}ClN_5O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			28	20	1	5	2		

- Molecule 4 is water.

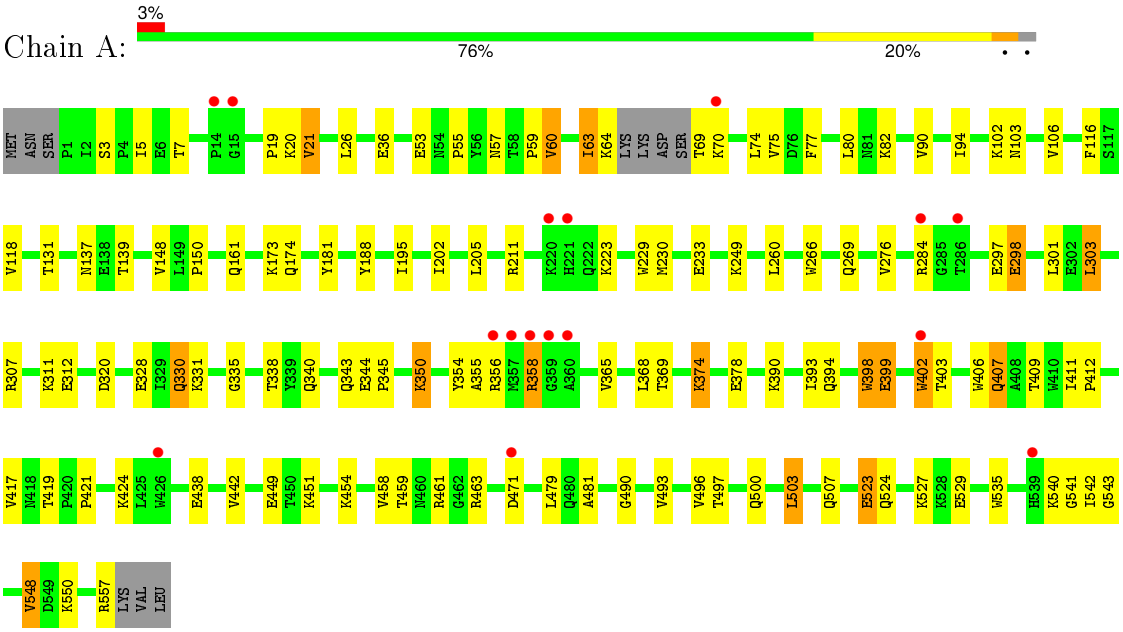
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	214	Total	O	0	0
			214	214		
4	B	148	Total	O	0	0
			148	148		

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.

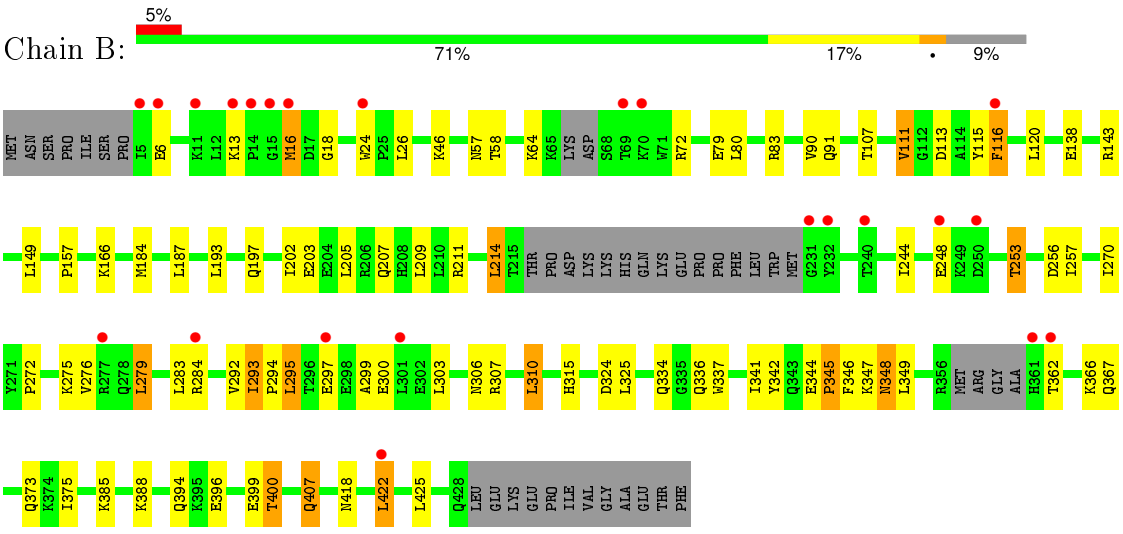
- Molecule 1: Reverse transcriptase/ribonuclease H

Chain A:



- Molecule 2: p51 RT

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	117.91Å 153.90Å 155.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.58 – 2.51 16.55 – 2.51	Depositor EDS
% Data completeness (in resolution range)	87.5 (16.58-2.51) 87.4 (16.55-2.51)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 2.52Å)	Xtriage
Refinement program	BUSTER 2.9.4	Depositor
R, R_{free}	0.193 , 0.249 0.194 , 0.254	Depositor DCC
R_{free} test set	2150 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	54.9	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 57.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 42363 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8227	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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

Bond lengths and bond angles in the following residue types are not validated in this section: M06

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	0.51	0/4619	0.76	0/6277
2	B	0.50	0/3427	0.74	1/4657 (0.0%)
All	All	0.50	0/8046	0.75	1/10934 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	345	PRO	N-CA-C	5.26	125.78	112.10

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	4503	0	4547	48	0
2	B	3334	0	3355	39	0
3	A	28	0	14	2	0
4	A	214	0	0	1	0
4	B	148	0	0	0	0
All	All	8227	0	7916	83	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 5.

All (83) 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)
2:B:79:GLU:HG3	2:B:83:ARG:HE	1.49	0.76
2:B:396:GLU:O	2:B:400:THR:HG22	1.87	0.74
1:A:330:GLN:HE22	1:A:340:GLN:HE22	1.36	0.71
1:A:298:GLU:CD	1:A:298:GLU:H	1.91	0.71
2:B:214:LEU:HD23	2:B:214:LEU:H	1.56	0.70
1:A:103:ASN:H	3:A:561:M06:HN14	1.37	0.70
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.26	0.69
2:B:337:TRP:HE1	2:B:367:GLN:HE21	1.38	0.69
2:B:207:GLN:HE21	2:B:211:ARG:HH12	1.40	0.68
1:A:298:GLU:N	1:A:298:GLU:OE2	2.29	0.65
2:B:207:GLN:NE2	2:B:211:ARG:HH12	1.94	0.65
1:A:63:ILE:HG21	1:A:74:LEU:HD12	1.80	0.63
1:A:297:GLU:HB3	1:A:298:GLU:OE2	2.01	0.60
1:A:57:ASN:ND2	1:A:131:THR:OG1	2.35	0.59
1:A:181:TYR:HB2	1:A:188:TYR:HB2	1.87	0.56
1:A:354:TYR:HD1	1:A:374:LYS:HD3	1.71	0.55
2:B:295:LEU:HD23	2:B:300:GLU:HG3	1.90	0.54
1:A:330:GLN:HE22	1:A:340:GLN:NE2	2.05	0.54
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.88	0.54
2:B:275:LYS:H	2:B:306:ASN:HD21	1.54	0.54
1:A:21:VAL:HG22	1:A:59:PRO:HD3	1.90	0.54
1:A:330:GLN:NE2	1:A:340:GLN:HE22	2.07	0.53
2:B:362:THR:CG2	2:B:367:GLN:HG3	2.39	0.52
1:A:369:THR:HG22	1:A:411:ILE:HD11	1.90	0.52
1:A:438:GLU:HG3	1:A:461:ARG:HG2	1.91	0.52
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.91	0.52
2:B:362:THR:HG22	2:B:367:GLN:HG3	1.92	0.52
1:A:399:GLU:O	1:A:403:THR:HB	2.11	0.51
1:A:320:ASP:O	1:A:343:GLN:NE2	2.44	0.51
1:A:3:SER:OG	1:A:5:ILE:HG13	2.12	0.50
1:A:399:GLU:HA	1:A:402:TRP:HE3	1.77	0.49
1:A:417:VAL:HG22	1:A:419:THR:HG23	1.95	0.49
2:B:244:ILE:HB	2:B:310:LEU:HG	1.95	0.49
1:A:298:GLU:HA	1:A:301:LEU:HD12	1.94	0.48
1:A:181:TYR:CD1	2:B:138:GLU:HA	2.48	0.48
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.95	0.48
1:A:458:VAL:HG22	1:A:548:VAL:HG22	1.96	0.48
1:A:229:TRP:CE2	1:A:230:MET:HG2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:253:THR:HG22	2:B:256:ASP:H	1.79	0.48
2:B:325:LEU:HD12	2:B:385:LYS:HB3	1.96	0.47
2:B:344:GLU:HB3	2:B:347:LYS:HE2	1.96	0.47
2:B:279:LEU:HD22	2:B:299:ALA:HB1	1.95	0.47
2:B:342:TYR:HB3	2:B:348:ASN:HB3	1.97	0.47
1:A:365:VAL:O	1:A:369:THR:HG23	2.15	0.47
1:A:77:PHE:CE2	1:A:150:PRO:HB2	2.49	0.46
1:A:331:LYS:HB3	1:A:421:PRO:HG2	1.98	0.46
2:B:107:THR:HG21	2:B:202:ILE:HD13	1.98	0.46
2:B:24:TRP:N	2:B:24:TRP:CD1	2.83	0.45
2:B:373:GLN:HE22	2:B:407:GLN:H	1.63	0.45
1:A:303:LEU:O	1:A:307:ARG:HG3	2.16	0.44
1:A:20:LYS:HE2	1:A:55:PRO:HB2	1.98	0.44
2:B:303:LEU:HD13	2:B:307:ARG:HH21	1.82	0.44
2:B:13:LYS:HB2	2:B:16:MET:CE	2.48	0.44
2:B:272:PRO:HG2	2:B:315:HIS:HB3	1.98	0.44
1:A:350:LYS:HE2	1:A:378:GLU:OE2	2.18	0.44
1:A:540:LYS:O	1:A:542:ILE:N	2.47	0.44
1:A:497:THR:O	1:A:535:TRP:HA	2.17	0.44
1:A:82:LYS:HD3	4:A:668:HOH:O	2.18	0.44
2:B:111:VAL:HG21	2:B:187:LEU:HD22	2.00	0.43
1:A:60:VAL:HG13	1:A:75:VAL:HG22	2.00	0.43
2:B:157:PRO:HG3	2:B:184:MET:HA	1.99	0.43
2:B:193:LEU:HB3	2:B:197:GLN:HB2	2.01	0.43
1:A:500:GLN:HG3	2:B:422:LEU:HD12	2.00	0.43
1:A:297:GLU:CB	1:A:298:GLU:OE2	2.67	0.42
2:B:57:ASN:OD1	2:B:143:ARG:NH1	2.52	0.42
1:A:407:GLN:HE22	2:B:394:GLN:HB2	1.83	0.42
2:B:293:ILE:HA	2:B:294:PRO:HD3	1.97	0.42
1:A:335:GLY:O	1:A:355:ALA:HA	2.19	0.41
1:A:266:TRP:O	1:A:269:GLN:HG2	2.20	0.41
2:B:24:TRP:CZ3	2:B:399:GLU:HG2	2.55	0.41
2:B:116:PHE:C	2:B:116:PHE:HD2	2.24	0.41
2:B:362:THR:HG23	2:B:366:LYS:HE3	2.02	0.41
2:B:324:ASP:HA	2:B:385:LYS:HE2	2.02	0.41
1:A:356:ARG:NH2	1:A:358:ARG:HD2	2.36	0.41
1:A:116:PHE:O	1:A:148:VAL:HG11	2.20	0.40
2:B:257:ILE:HG13	2:B:283:LEU:HD21	2.03	0.40
1:A:393:ILE:HD13	1:A:398:TRP:HD1	1.85	0.40
2:B:115:TYR:HB3	2:B:149:LEU:HB2	2.02	0.40
1:A:229:TRP:CD2	3:A:561:M06:H9	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:LEU:HD22	1:A:507:GLN:HG3	2.03	0.40
2:B:373:GLN:NE2	2:B:407:GLN:H	2.20	0.40
1:A:523:GLU:HG2	1:A:524:GLN:N	2.35	0.40
2:B:341:ILE:HD11	2:B:375:ILE:HG23	2.03	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	549/563 (98%)	520 (95%)	23 (4%)	6 (1%)	17	31
2	B	395/443 (89%)	378 (96%)	15 (4%)	2 (0%)	34	55
All	All	944/1006 (94%)	898 (95%)	38 (4%)	8 (1%)	24	41

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	VAL
1	A	412	PRO
1	A	541	GLY
1	A	543	GLY
2	B	345	PRO
1	A	345	PRO
1	A	490	GLY
2	B	18	GLY

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	493/503 (98%)	430 (87%)	63 (13%)	5 10
2	B	367/403 (91%)	327 (89%)	40 (11%)	8 15
All	All	860/906 (95%)	757 (88%)	103 (12%)	6 12

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	21	VAL
1	A	26	LEU
1	A	36	GLU
1	A	53	GLU
1	A	60	VAL
1	A	63	ILE
1	A	64	LYS
1	A	69	THR
1	A	70	LYS
1	A	94	ILE
1	A	102	LYS
1	A	106	VAL
1	A	118	VAL
1	A	137	ASN
1	A	139	THR
1	A	161	GLN
1	A	173	LYS
1	A	174	GLN
1	A	195	ILE
1	A	202	ILE
1	A	205	LEU
1	A	211	ARG
1	A	223	LYS
1	A	233	GLU
1	A	249	LYS
1	A	260	LEU
1	A	276	VAL
1	A	284	ARG
1	A	298	GLU
1	A	303	LEU
1	A	311	LYS
1	A	312	GLU

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Mol	Chain	Res	Type
1	A	330	GLN
1	A	338	THR
1	A	344	GLU
1	A	350	LYS
1	A	358	ARG
1	A	368	LEU
1	A	374	LYS
1	A	394	GLN
1	A	398	TRP
1	A	399	GLU
1	A	402	TRP
1	A	407	GLN
1	A	409	THR
1	A	424	LYS
1	A	449	GLU
1	A	451	LYS
1	A	454	LYS
1	A	459	THR
1	A	463	ARG
1	A	471	ASP
1	A	479	LEU
1	A	493	VAL
1	A	496	VAL
1	A	503	LEU
1	A	523	GLU
1	A	527	LYS
1	A	529	GLU
1	A	548	VAL
1	A	550	LYS
1	A	557	ARG
2	B	6	GLU
2	B	16	MET
2	B	26	LEU
2	B	46	LYS
2	B	58	THR
2	B	64	LYS
2	B	72	ARG
2	B	80	LEU
2	B	90	VAL
2	B	91	GLN
2	B	111	VAL
2	B	113	ASP

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Mol	Chain	Res	Type
2	B	116	PHE
2	B	120	LEU
2	B	166	LYS
2	B	203	GLU
2	B	205	LEU
2	B	209	LEU
2	B	214	LEU
2	B	248	GLU
2	B	253	THR
2	B	270	ILE
2	B	276	VAL
2	B	279	LEU
2	B	284	ARG
2	B	292	VAL
2	B	293	ILE
2	B	295	LEU
2	B	297	GLU
2	B	310	LEU
2	B	334	GLN
2	B	336	GLN
2	B	346	PHE
2	B	348	ASN
2	B	349	LEU
2	B	388	LYS
2	B	400	THR
2	B	407	GLN
2	B	422	LEU
2	B	425	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	137	ASN
1	A	147	ASN
1	A	198	HIS
1	A	222	GLN
1	A	235	HIS
1	A	258	GLN
1	A	330	GLN
1	A	407	GLN
1	A	474	ASN

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Mol	Chain	Res	Type
1	A	512	GLN
1	A	519	ASN
2	B	147	ASN
2	B	175	ASN
2	B	182	GLN
2	B	207	GLN
2	B	208	HIS
2	B	258	GLN
2	B	278	GLN
2	B	306	ASN
2	B	367	GLN
2	B	373	GLN
2	B	394	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

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	M06	A	561	-	30,31,31	2.12	9 (30%)	28,44,44	2.61	7 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	M06	A	561	-	-	0/9/10/10	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	561	M06	C10-CL	-2.07	1.69	1.74
3	A	561	M06	C1-C	2.24	1.44	1.39
3	A	561	M06	C20-C21	2.30	1.41	1.36
3	A	561	M06	C9-C8	2.77	1.44	1.39
3	A	561	M06	C9-C10	3.06	1.43	1.38
3	A	561	M06	C3-N	3.28	1.43	1.38
3	A	561	M06	C13-N14	3.79	1.38	1.33
3	A	561	M06	C19-N18	4.24	1.41	1.32
3	A	561	M06	C3-C4	5.52	1.55	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	561	M06	C13-C22-N	-10.72	98.43	111.60
3	A	561	M06	C21-C20-C19	-2.53	115.28	118.88
3	A	561	M06	C19-N18-C16	-2.11	113.71	116.44
3	A	561	M06	C5-O-C4	2.15	122.21	118.47
3	A	561	M06	C20-C19-N18	2.42	127.74	123.94
3	A	561	M06	C1-C2-N	3.37	124.23	121.32
3	A	561	M06	C6-C-C4	4.40	125.55	120.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	561	M06	2	0

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	553/563 (98%)	0.02	16 (2%)	55	60	33, 59, 89, 107	0
2	B	403/443 (90%)	0.09	23 (5%)	27	31	37, 59, 100, 117	0
All	All	956/1006 (95%)	0.05	39 (4%)	41	46	33, 59, 95, 117	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	15	GLY	5.3
2	B	361	HIS	5.2
2	B	362	THR	4.9
1	A	358	ARG	4.6
2	B	70	LYS	4.5
2	B	231	GLY	4.4
1	A	286	THR	4.3
2	B	14	PRO	4.3
2	B	297	GLU	4.2
2	B	69	THR	3.8
2	B	301	LEU	3.8
1	A	359	GLY	3.8
2	B	250	ASP	3.4
1	A	360	ALA	3.2
2	B	248	GLU	3.1
2	B	232	TYR	3.1
2	B	284	ARG	3.1
2	B	11	LYS	3.0
2	B	116	PHE	3.0
2	B	240	THR	2.9
1	A	284	ARG	2.8
2	B	277	ARG	2.7
1	A	539	HIS	2.6
2	B	24	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	5	ILE	2.4
1	A	220	LYS	2.4
1	A	15	GLY	2.3
2	B	13	LYS	2.3
2	B	16	MET	2.3
1	A	14	PRO	2.3
1	A	357	MET	2.3
1	A	426	TRP	2.3
1	A	356	ARG	2.2
2	B	6	GLU	2.2
1	A	402	TRP	2.1
1	A	70	LYS	2.1
1	A	221	HIS	2.0
1	A	471	ASP	2.0
2	B	422	LEU	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	M06	A	561	28/28	0.97	0.10	-0.88	38,52,59,60	0

6.5 Other polymers (i)

There are no such residues in this entry.