Full wwPDB X-ray Structure Validation Report ⓘ

Jan 14, 2024 – 07:16 am GMT

PDB ID	:	6TOQ
Title	:	Crystal structure of a PP2A B56y/HTLV-1 integrase complex
Authors	:	Minnell, J.J.; Barski, M.S.; Maertens, G.N.
Deposited on	:	2019-12-11
Resolution	:	3.16 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:

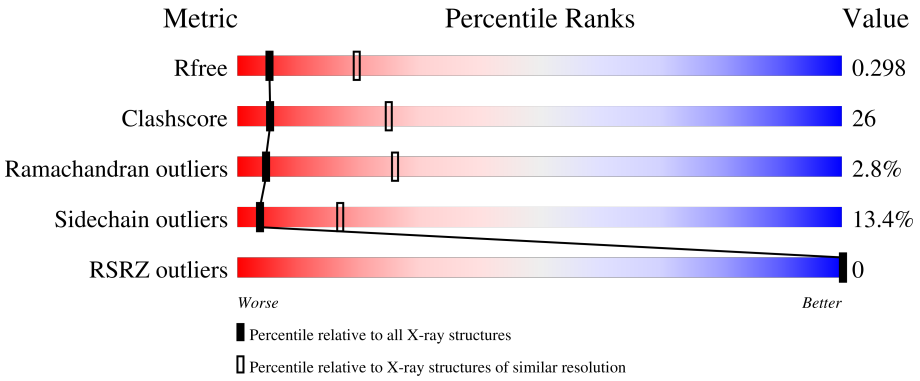
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.16 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	CCC	98	93%
2	AAA	370	45% 36% 7% 11%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2720 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 Pol protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	CCC	7	45	31	7	7	0	0	0

- Molecule 2 is a protein called Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	AAA	329	2629	1738	417	462	12	0	0	0

- Molecule 3 is water.

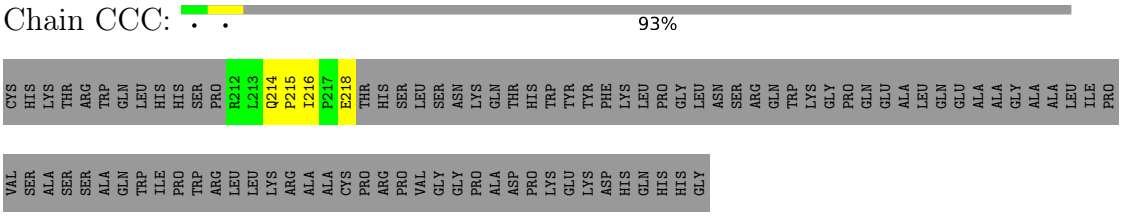
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	CCC	4	4	4	0	0
			Total	O		
3	AAA	42	42	42	0	0

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.

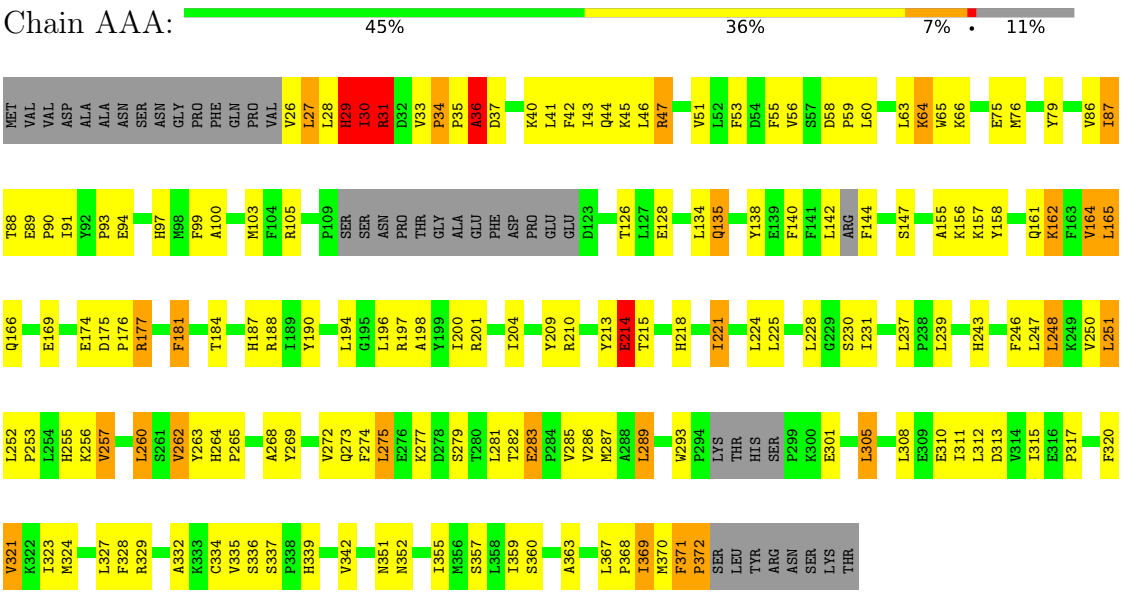
• Molecule 1: Pol protein

Chain CCC:



• Molecule 2: Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform

Chain AAA:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	58.77Å 58.77Å 321.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.29 – 3.16 80.29 – 3.16	Depositor EDS
% Data completeness (in resolution range)	95.9 (80.29-3.16) 88.4 (80.29-3.16)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.227 , 0.294 0.221 , 0.298	Depositor DCC
R_{free} test set	537 reflections (5.35%)	wwPDB-VP
Wilson B-factor (Å^2)	62.7	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 85.8	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	0.91	EDS
Total number of atoms	2720	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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	CCC	0.42	0/46	0.85	0/64
2	AAA	0.40	0/2697	0.86	3/3674 (0.1%)
All	All	0.40	0/2743	0.86	3/3738 (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
2	AAA	0	5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AAA	310	GLU	CB-CA-C	6.13	122.67	110.40
2	AAA	329	ARG	CB-CA-C	5.56	121.52	110.40
2	AAA	177	ARG	CB-CA-C	5.04	120.47	110.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AAA	218	HIS	Peptide
2	AAA	31	ARG	Peptide
2	AAA	34	PRO	Peptide
2	AAA	36	ALA	Peptide
2	AAA	369	ILE	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	CCC	45	0	41	5	0
2	AAA	2629	0	2582	137	0
3	AAA	42	0	0	3	0
3	CCC	4	0	0	0	0
All	All	2720	0	2623	139	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 26.

All (139) 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:AAA:34:PRO:HD3	2:AAA:75:GLU:OE2	1.52	1.07
2:AAA:363:ALA:HB1	2:AAA:367:LEU:HD22	1.47	0.97
2:AAA:287:MET:CE	2:AAA:323:ILE:HG22	2.01	0.91
2:AAA:287:MET:HE1	2:AAA:323:ILE:HG22	1.55	0.88
2:AAA:312:LEU:O	2:AAA:315:ILE:HG22	1.76	0.84
2:AAA:281:LEU:O	2:AAA:285:VAL:HG23	1.78	0.83
2:AAA:87:ILE:HA	2:AAA:91:ILE:HD11	1.62	0.81
2:AAA:371:PHE:CB	2:AAA:372:PRO:HD2	2.11	0.80
2:AAA:142:LEU:C	2:AAA:144:PHE:N	2.36	0.79
1:CCC:215:PRO:HA	2:AAA:230:SER:HB2	1.66	0.76
2:AAA:255:HIS:HA	2:AAA:260:LEU:HD12	1.65	0.75
2:AAA:26:VAL:HA	2:AAA:65:TRP:CH2	2.22	0.75
2:AAA:209:TYR:CB	3:AAA:416:HOH:O	2.36	0.72
2:AAA:103:MET:HE3	2:AAA:103:MET:HA	1.69	0.72
2:AAA:27:LEU:O	2:AAA:27:LEU:HG	1.89	0.72
2:AAA:269:TYR:CE2	2:AAA:273:GLN:HG3	2.24	0.71
2:AAA:29:HIS:O	2:AAA:30:ILE:HG13	1.90	0.71
2:AAA:60:LEU:O	2:AAA:63:LEU:HD21	1.90	0.70
2:AAA:29:HIS:C	2:AAA:30:ILE:HG13	2.11	0.70
2:AAA:194:LEU:HD22	2:AAA:194:LEU:H	1.55	0.70
2:AAA:255:HIS:HA	2:AAA:260:LEU:CD1	2.23	0.68
2:AAA:103:MET:O	2:AAA:105:ARG:NH1	2.28	0.66
2:AAA:31:ARG:HH12	2:AAA:45:LYS:HA	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AAA:31:ARG:NH1	2:AAA:45:LYS:HA	2.12	0.64
2:AAA:210:ARG:HA	2:AAA:214:GLU:HB2	1.77	0.64
2:AAA:221:ILE:H	2:AAA:221:ILE:HD13	1.63	0.64
2:AAA:355:ILE:O	2:AAA:359:ILE:HG13	1.97	0.63
2:AAA:79:TYR:CE2	2:AAA:86:VAL:HG11	2.33	0.63
2:AAA:286:VAL:HG11	2:AAA:323:ILE:HD13	1.80	0.63
2:AAA:327:LEU:O	2:AAA:327:LEU:HD23	1.99	0.62
2:AAA:162:LYS:H	2:AAA:162:LYS:HD2	1.64	0.62
2:AAA:279:SER:O	2:AAA:282:THR:HG23	2.00	0.62
2:AAA:363:ALA:O	2:AAA:367:LEU:HB2	2.00	0.61
2:AAA:93:PRO:HB3	2:AAA:158:TYR:CE2	2.36	0.60
2:AAA:221:ILE:O	2:AAA:225:LEU:HB2	2.02	0.59
2:AAA:43:ILE:HD11	2:AAA:91:ILE:HG22	1.84	0.59
2:AAA:103:MET:HA	2:AAA:103:MET:CE	2.32	0.58
2:AAA:275:LEU:HG	2:AAA:282:THR:HG22	1.84	0.58
2:AAA:246:PHE:CE2	2:AAA:251:LEU:HD13	2.38	0.58
2:AAA:352:ASN:HB3	2:AAA:355:ILE:HB	1.85	0.58
2:AAA:246:PHE:CE1	2:AAA:250:VAL:HG11	2.40	0.57
1:CCC:216:ILE:HD11	2:AAA:187:HIS:CD2	2.40	0.56
2:AAA:60:LEU:O	2:AAA:63:LEU:CD2	2.54	0.55
2:AAA:89:GLU:N	2:AAA:90:PRO:HD2	2.22	0.55
2:AAA:367:LEU:N	2:AAA:368:PRO:CD	2.71	0.54
2:AAA:142:LEU:O	2:AAA:144:PHE:N	2.41	0.54
2:AAA:248:LEU:HD12	2:AAA:252:LEU:HD11	1.90	0.54
2:AAA:257:VAL:HG22	2:AAA:263:TYR:OH	2.07	0.54
2:AAA:289:LEU:HD13	2:AAA:308:LEU:CD2	2.39	0.53
2:AAA:268:ALA:O	2:AAA:272:VAL:HG23	2.09	0.53
2:AAA:138:TYR:HB3	2:AAA:181:PHE:CG	2.44	0.53
2:AAA:27:LEU:HD22	2:AAA:65:TRP:CG	2.45	0.52
2:AAA:103:MET:SD	2:AAA:138:TYR:CE1	3.03	0.52
2:AAA:135:GLN:O	2:AAA:135:GLN:HG3	2.03	0.51
2:AAA:99:PHE:CZ	2:AAA:103:MET:HG3	2.44	0.51
2:AAA:213:TYR:O	2:AAA:215:THR:N	2.43	0.51
2:AAA:327:LEU:HD23	2:AAA:327:LEU:C	2.30	0.51
2:AAA:64:LYS:HD3	2:AAA:64:LYS:H	1.75	0.51
2:AAA:252:LEU:HB2	2:AAA:253:PRO:HD3	1.92	0.51
2:AAA:287:MET:HE2	2:AAA:323:ILE:HG22	1.90	0.51
2:AAA:371:PHE:CB	2:AAA:372:PRO:CD	2.84	0.51
2:AAA:332:ALA:O	2:AAA:335:VAL:HG22	2.11	0.50
2:AAA:59:PRO:O	2:AAA:66:LYS:NZ	2.44	0.50
2:AAA:30:ILE:O	2:AAA:31:ARG:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AAA:324:MET:O	2:AAA:328:PHE:HD2	1.93	0.49
2:AAA:260:LEU:O	2:AAA:264:HIS:HB2	2.11	0.49
2:AAA:289:LEU:HD13	2:AAA:308:LEU:HD22	1.95	0.49
2:AAA:43:ILE:CG2	2:AAA:47:ARG:HH11	2.26	0.49
2:AAA:260:LEU:HD21	2:AAA:264:HIS:ND1	2.28	0.49
2:AAA:27:LEU:HD23	2:AAA:28:LEU:HD22	1.94	0.49
2:AAA:27:LEU:HD22	2:AAA:65:TRP:CD2	2.47	0.49
2:AAA:283:GLU:O	2:AAA:287:MET:HG2	2.13	0.49
2:AAA:339:HIS:O	2:AAA:342:VAL:HB	2.12	0.49
2:AAA:43:ILE:CD1	2:AAA:91:ILE:HG22	2.42	0.48
2:AAA:336:SER:O	2:AAA:337:SER:C	2.51	0.48
2:AAA:214:GLU:OE2	2:AAA:214:GLU:HA	2.14	0.48
2:AAA:93:PRO:HB3	2:AAA:158:TYR:CD2	2.48	0.48
1:CCC:216:ILE:O	1:CCC:218:GLU:N	2.44	0.48
2:AAA:293:TRP:HE1	2:AAA:301:GLU:HG2	1.77	0.48
2:AAA:248:LEU:HA	2:AAA:252:LEU:HD12	1.97	0.47
2:AAA:46:LEU:HD23	2:AAA:76:MET:SD	2.55	0.47
2:AAA:213:TYR:C	2:AAA:215:THR:N	2.68	0.46
2:AAA:275:LEU:HD11	2:AAA:285:VAL:HG21	1.97	0.46
2:AAA:359:ILE:O	2:AAA:363:ALA:N	2.49	0.46
2:AAA:194:LEU:H	2:AAA:194:LEU:CD2	2.25	0.46
2:AAA:29:HIS:C	2:AAA:30:ILE:CG1	2.82	0.46
2:AAA:35:PRO:O	2:AAA:36:ALA:HB2	2.16	0.46
2:AAA:126:THR:HB	2:AAA:174:GLU:OE1	2.15	0.46
2:AAA:138:TYR:HB3	2:AAA:181:PHE:CD2	2.51	0.46
2:AAA:204:ILE:HD13	2:AAA:224:LEU:HD22	1.98	0.45
2:AAA:315:ILE:HG12	2:AAA:320:PHE:HB2	1.97	0.45
2:AAA:164:VAL:HG21	2:AAA:196:LEU:HD13	1.98	0.45
2:AAA:213:TYR:C	2:AAA:215:THR:H	2.19	0.45
2:AAA:128:GLU:HG2	2:AAA:134:LEU:HD12	1.98	0.45
2:AAA:200:ILE:O	2:AAA:201:ARG:C	2.55	0.45
2:AAA:34:PRO:HB3	2:AAA:41:LEU:HD23	1.98	0.44
2:AAA:97:HIS:O	2:AAA:100:ALA:HB3	2.17	0.44
2:AAA:253:PRO:O	2:AAA:256:LYS:HG2	2.17	0.44
2:AAA:43:ILE:HG22	2:AAA:47:ARG:HH11	1.82	0.43
2:AAA:273:GLN:O	2:AAA:277:LYS:HG2	2.17	0.43
2:AAA:29:HIS:HB3	2:AAA:30:ILE:H	1.52	0.43
2:AAA:87:ILE:HA	2:AAA:91:ILE:CD1	2.39	0.43
2:AAA:247:LEU:HD22	2:AAA:274:PHE:CD2	2.53	0.43
2:AAA:42:PHE:HE1	2:AAA:76:MET:HG2	1.84	0.43
2:AAA:264:HIS:N	2:AAA:265:PRO:HD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AAA:370:MET:HG3	2:AAA:370:MET:O	2.19	0.43
2:AAA:28:LEU:O	2:AAA:29:HIS:HB2	2.17	0.43
2:AAA:275:LEU:HD23	2:AAA:311:ILE:HG23	1.99	0.43
1:CCC:214:GLN:HA	1:CCC:215:PRO:HD3	1.91	0.42
2:AAA:239:LEU:HD22	2:AAA:243:HIS:HB2	2.01	0.42
2:AAA:317:PRO:O	2:AAA:321:VAL:HG22	2.19	0.42
2:AAA:88:THR:C	2:AAA:90:PRO:HD2	2.39	0.42
2:AAA:228:LEU:HD23	2:AAA:231:ILE:HD12	2.00	0.42
2:AAA:51:VAL:HG12	2:AAA:53:PHE:CE1	2.55	0.42
2:AAA:257:VAL:CG2	2:AAA:263:TYR:OH	2.68	0.42
2:AAA:175:ASP:HA	2:AAA:176:PRO:HD3	1.86	0.42
2:AAA:260:LEU:HA	2:AAA:263:TYR:CE2	2.55	0.42
2:AAA:264:HIS:N	2:AAA:265:PRO:CD	2.83	0.42
2:AAA:269:TYR:CE2	2:AAA:273:GLN:CG	3.01	0.42
2:AAA:34:PRO:HD3	2:AAA:75:GLU:CD	2.34	0.42
2:AAA:33:VAL:C	2:AAA:35:PRO:HD3	2.40	0.41
2:AAA:55:PHE:HD2	3:AAA:407:HOH:O	2.02	0.41
2:AAA:305:LEU:HD13	2:AAA:305:LEU:HA	1.89	0.41
2:AAA:190:TYR:CE2	2:AAA:197:ARG:HD3	2.55	0.41
2:AAA:165:LEU:HD23	2:AAA:166:GLN:HG2	2.01	0.41
2:AAA:166:GLN:HA	2:AAA:169:GLU:HB2	2.02	0.41
2:AAA:262:VAL:HG12	2:AAA:263:TYR:HD2	1.85	0.41
2:AAA:34:PRO:CD	2:AAA:75:GLU:OE2	2.44	0.41
2:AAA:42:PHE:CE1	2:AAA:76:MET:HG2	2.56	0.41
2:AAA:76:MET:HB3	2:AAA:140:PHE:CE1	2.56	0.41
2:AAA:155:ALA:C	2:AAA:157:LYS:N	2.75	0.40
2:AAA:161:GLN:HG3	3:AAA:405:HOH:O	2.20	0.40
2:AAA:93:PRO:HD3	2:AAA:158:TYR:CZ	2.57	0.40
2:AAA:194:LEU:HA	2:AAA:197:ARG:HG3	2.04	0.40
1:CCC:216:ILE:HG21	2:AAA:190:TYR:CD2	2.57	0.40
2:AAA:334:CYS:O	2:AAA:337:SER:HB3	2.21	0.40
2:AAA:43:ILE:HD12	2:AAA:94:GLU:HG3	2.04	0.40
2:AAA:214:GLU:OE2	2:AAA:214:GLU:CA	2.70	0.40
2:AAA:315:ILE:HD11	2:AAA:320:PHE:HA	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	CCC	5/98 (5%)	4 (80%)	1 (20%)	0	100 100
2	AAA	321/370 (87%)	282 (88%)	30 (9%)	9 (3%)	5 26
All	All	326/468 (70%)	286 (88%)	31 (10%)	9 (3%)	5 26

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AAA	36	ALA
2	AAA	371	PHE
2	AAA	29	HIS
2	AAA	214	GLU
2	AAA	58	ASP
2	AAA	198	ALA
2	AAA	156	LYS
2	AAA	369	ILE
2	AAA	30	ILE

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	CCC	4/82 (5%)	4 (100%)	0	100 100
2	AAA	280/343 (82%)	242 (86%)	38 (14%)	3 16
All	All	284/425 (67%)	246 (87%)	38 (13%)	4 17

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AAA	27	LEU
2	AAA	29	HIS
2	AAA	30	ILE
2	AAA	31	ARG
2	AAA	37	ASP
2	AAA	40	LYS
2	AAA	44	GLN
2	AAA	47	ARG
2	AAA	56	VAL
2	AAA	64	LYS
2	AAA	87	ILE
2	AAA	135	GLN
2	AAA	147	SER
2	AAA	162	LYS
2	AAA	164	VAL
2	AAA	165	LEU
2	AAA	177	ARG
2	AAA	181	PHE
2	AAA	184	THR
2	AAA	188	ARG
2	AAA	214	GLU
2	AAA	221	ILE
2	AAA	237	LEU
2	AAA	248	LEU
2	AAA	251	LEU
2	AAA	257	VAL
2	AAA	260	LEU
2	AAA	262	VAL
2	AAA	275	LEU
2	AAA	283	GLU
2	AAA	289	LEU
2	AAA	305	LEU
2	AAA	313	ASP
2	AAA	321	VAL
2	AAA	351	ASN
2	AAA	357	SER
2	AAA	360	SER
2	AAA	372	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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	CCC	7/98 (7%)	0.43	0	100	100	72, 80, 101, 114	0
2	AAA	329/370 (88%)	-0.24	0	100	100	37, 58, 86, 113	0
All	All	336/468 (71%)	-0.22	0	100	100	37, 59, 89, 114	0

There are no RSRZ outliers to report.

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.