Full wwPDB X-ray Structure Validation Report (i)

Apr 10, 2023 – 08:56 PM EDT

PDB ID	:	1A6C
Title	:	STRUCTURE OF TOBACCO RINGSPOT VIRUS
Authors	:	Johnson, J.E.; Chandrasekar, V.
Deposited on	:	1998-02-23
Resolution	:	3.50 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:

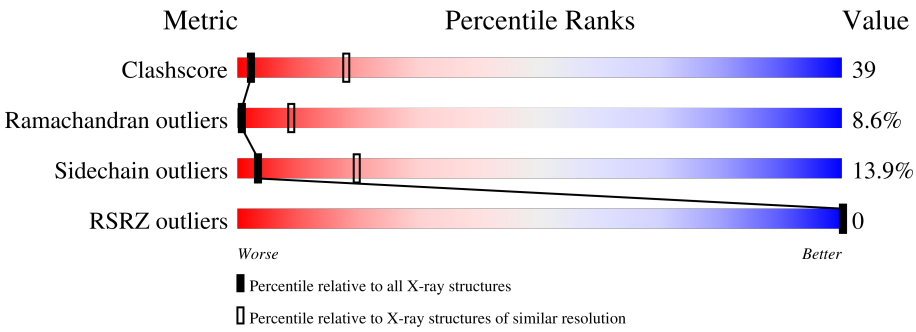
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 3.50 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	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	513	47% 38% 11% •

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4016 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 TOBACCO RINGSPOT VIRUS CAPSID PROTEIN.

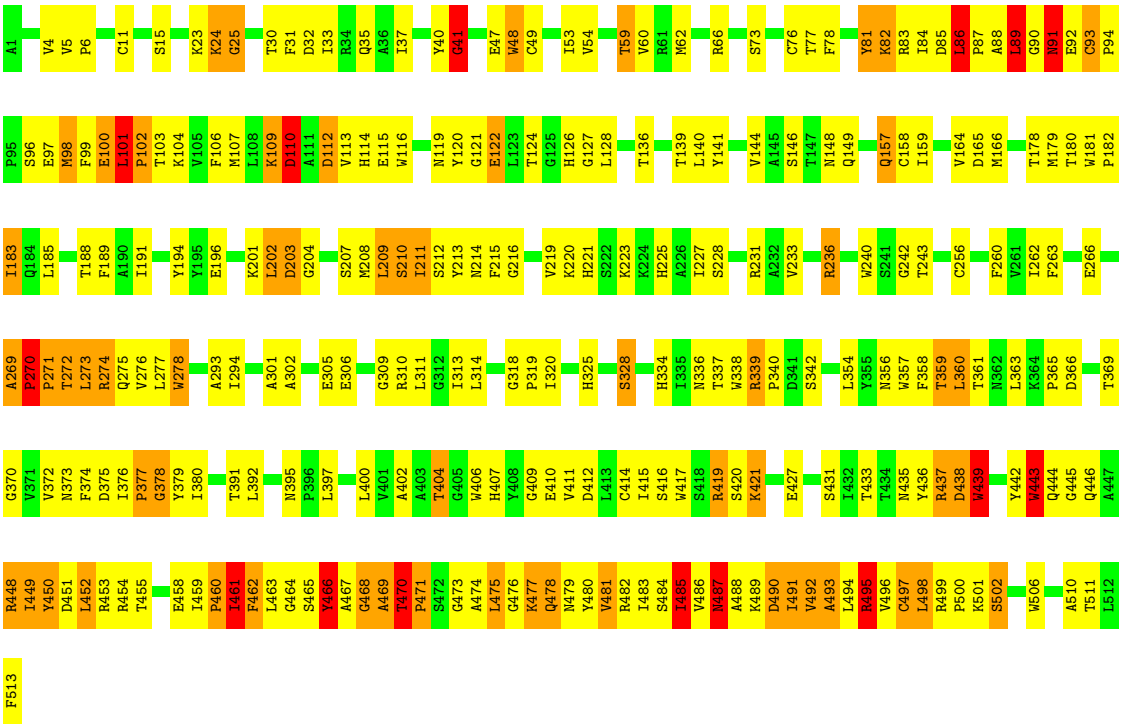
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	513	4016	2575	683	735	23	0	0	0

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: TOBACCO RINGSPOT VIRUS CAPSID PROTEIN

Chain A: 47% 38% 11% •



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	407.06Å 399.68Å 285.97Å 90.00° 129.10° 90.00°	Depositor
Resolution (Å)	8.00 – 3.50 49.50 – 2.99	Depositor EDS
% Data completeness (in resolution range)	27.5 (8.00-3.50) 13.0 (49.50-2.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	8.69 (at 3.01Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.269 , (Not available) 0.261 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	35.2	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 8.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.75	EDS
Total number of atoms	4016	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% 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	0.54	0/4136	0.87	12/5635 (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	2

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	451	ASP	N-CA-C	-9.52	85.30	111.00
1	A	82	LYS	N-CA-C	7.38	130.91	111.00
1	A	485	ILE	N-CA-C	-7.36	91.13	111.00
1	A	492	VAL	N-CA-C	-6.85	92.50	111.00
1	A	461	ILE	N-CA-C	6.77	129.28	111.00
1	A	495	ARG	N-CA-C	-5.98	94.84	111.00
1	A	100	GLU	N-CA-C	-5.81	95.32	111.00
1	A	360	LEU	CA-CB-CG	5.80	128.63	115.30
1	A	270	PRO	N-CA-C	-5.78	97.07	112.10
1	A	101	LEU	CA-CB-CG	5.67	128.35	115.30
1	A	210	SER	N-CA-C	-5.11	97.20	111.00
1	A	41	GLY	N-CA-C	5.08	125.80	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	450	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	466	TYR	Sidechain

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	4016	0	3909	311	0
All	All	4016	0	3909	311	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 39.

All (311) 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:208:MET:HB2	1:A:313:ILE:HB	1.25	1.08
1:A:209:LEU:HD11	1:A:310:ARG:HB2	1.37	1.06
1:A:433:THR:HG22	1:A:445:GLY:HA3	1.39	1.02
1:A:110:ASP:HB2	1:A:113:VAL:HB	1.45	0.99
1:A:11:CYS:SG	1:A:37:ILE:HG12	2.04	0.96
1:A:213:TYR:HB3	1:A:301:ALA:HB1	1.50	0.93
1:A:482:ARG:NH2	1:A:494:LEU:HG	1.86	0.90
1:A:482:ARG:HH22	1:A:494:LEU:HG	1.39	0.88
1:A:76:CYS:O	1:A:102:PRO:HD2	1.76	0.85
1:A:372:VAL:HG23	1:A:486:VAL:HG21	1.59	0.84
1:A:485:ILE:HD13	1:A:485:ILE:H	1.44	0.83
1:A:11:CYS:HB2	1:A:164:VAL:HG23	1.60	0.83
1:A:485:ILE:HG12	1:A:489:LYS:HG3	1.60	0.83
1:A:427:GLU:HG3	1:A:485:ILE:HD11	1.60	0.80
1:A:48:TRP:CH2	1:A:128:LEU:HG	2.15	0.80
1:A:365:PRO:HA	1:A:372:VAL:HG22	1.65	0.78
1:A:98:MET:SD	1:A:231:ARG:NH1	2.58	0.76
1:A:15:SER:HB3	1:A:159:ILE:HG12	1.67	0.76
1:A:110:ASP:HB2	1:A:113:VAL:CB	2.16	0.76
1:A:48:TRP:HH2	1:A:128:LEU:HG	1.49	0.75
1:A:110:ASP:CB	1:A:113:VAL:HB	2.16	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:TRP:HB2	1:A:506:TRP:HB2	1.68	0.74
1:A:88:ALA:HA	1:A:223:LYS:HE2	1.69	0.74
1:A:213:TYR:HB3	1:A:301:ALA:CB	2.17	0.74
1:A:478:GLN:H	1:A:478:GLN:NE2	1.84	0.74
1:A:461:ILE:HG21	1:A:469:ALA:CB	2.18	0.73
1:A:93:CYS:HB3	1:A:94:PRO:HD3	1.70	0.73
1:A:77:THR:HG21	1:A:83:ARG:NH1	2.04	0.73
1:A:188:THR:HG22	1:A:339:ARG:HG3	1.68	0.73
1:A:379:TYR:HD2	1:A:469:ALA:HB2	1.53	0.72
1:A:24:LYS:O	1:A:144:VAL:HB	1.89	0.72
1:A:454:ARG:HD2	1:A:455:THR:H	1.53	0.72
1:A:419:ARG:HH21	1:A:484:SER:HB2	1.57	0.70
1:A:93:CYS:HB3	1:A:94:PRO:CD	2.21	0.69
1:A:164:VAL:HG12	1:A:165:ASP:H	1.58	0.69
1:A:109:LYS:O	1:A:110:ASP:HB3	1.92	0.69
1:A:66:ARG:CZ	1:A:109:LYS:HA	2.23	0.68
1:A:461:ILE:HG21	1:A:469:ALA:HB1	1.75	0.68
1:A:449:ILE:HD13	1:A:449:ILE:N	2.08	0.68
1:A:365:PRO:CA	1:A:372:VAL:HG22	2.24	0.67
1:A:83:ARG:HD2	1:A:99:PHE:HE2	1.59	0.67
1:A:482:ARG:HH12	1:A:494:LEU:H	1.43	0.66
1:A:442:TYR:O	1:A:443:TRP:HB3	1.94	0.66
1:A:435:ASN:HB3	1:A:477:LYS:HE3	1.77	0.66
1:A:89:LEU:HD22	1:A:90:GLY:N	2.11	0.66
1:A:419:ARG:NH2	1:A:484:SER:HB2	2.12	0.65
1:A:439:TRP:HA	1:A:439:TRP:CE3	2.32	0.65
1:A:409:GLY:O	1:A:460:PRO:HD2	1.97	0.64
1:A:410:GLU:O	1:A:501:LYS:HB2	1.97	0.64
1:A:378:GLY:O	1:A:460:PRO:HA	1.97	0.64
1:A:62:MET:O	1:A:114:HIS:HB2	1.97	0.64
1:A:220:LYS:HG3	1:A:225:HIS:CD2	2.33	0.63
1:A:379:TYR:CD2	1:A:469:ALA:HB2	2.33	0.63
1:A:482:ARG:HB2	1:A:486:VAL:HG22	1.81	0.63
1:A:276:VAL:HG21	1:A:314:LEU:HD22	1.80	0.62
1:A:81:TYR:CE2	1:A:136:THR:HG22	2.35	0.62
1:A:436:TYR:OH	1:A:473:GLY:HA2	1.99	0.62
1:A:202:LEU:O	1:A:203:ASP:HB2	2.00	0.62
1:A:416:SER:O	1:A:494:LEU:HA	2.00	0.62
1:A:466:TYR:HD1	1:A:466:TYR:O	1.83	0.62
1:A:475:LEU:HG	1:A:476:GLY:N	2.15	0.62
1:A:73:SER:OG	1:A:146:SER:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:ARG:CZ	1:A:493:ALA:HB1	2.31	0.61
1:A:485:ILE:HG13	1:A:489:LYS:HZ2	1.64	0.61
1:A:411:VAL:HG12	1:A:500:PRO:HA	1.82	0.61
1:A:363:LEU:HD13	1:A:374:PHE:CE1	2.36	0.61
1:A:92:GLU:O	1:A:93:CYS:HB2	2.01	0.60
1:A:269:ALA:O	1:A:271:PRO:HD3	2.02	0.60
1:A:446:GLN:HE22	1:A:454:ARG:HH21	1.49	0.60
1:A:89:LEU:HD22	1:A:90:GLY:H	1.67	0.60
1:A:86:LEU:N	1:A:86:LEU:HD13	2.16	0.60
1:A:412:ASP:HB2	1:A:499:ARG:CG	2.32	0.60
1:A:86:LEU:HD13	1:A:86:LEU:H	1.66	0.60
1:A:30:THR:HG22	1:A:141:TYR:HD1	1.67	0.60
1:A:263:PHE:CZ	1:A:270:PRO:HG3	2.37	0.60
1:A:201:LYS:HB2	1:A:328:SER:HB3	1.84	0.59
1:A:412:ASP:HB2	1:A:499:ARG:CD	2.32	0.59
1:A:47:GLU:OE1	1:A:166:MET:HG3	2.02	0.59
1:A:209:LEU:HD13	1:A:311:LEU:O	2.01	0.59
1:A:91:ASN:N	1:A:91:ASN:HD22	2.00	0.59
1:A:358:PHE:HB3	1:A:392:LEU:HD23	1.84	0.59
1:A:210:SER:O	1:A:212:SER:N	2.36	0.59
1:A:212:SER:HB3	1:A:213:TYR:CE2	2.38	0.59
1:A:437:ARG:HD3	1:A:442:TYR:CE2	2.38	0.59
1:A:449:ILE:HD13	1:A:449:ILE:H	1.67	0.59
1:A:485:ILE:O	1:A:489:LYS:HG3	2.03	0.59
1:A:397:LEU:HD23	1:A:498:LEU:HD13	1.83	0.58
1:A:77:THR:HG22	1:A:141:TYR:HB2	1.85	0.58
1:A:164:VAL:HG12	1:A:165:ASP:N	2.17	0.58
1:A:120:TYR:CE1	1:A:128:LEU:HB2	2.38	0.58
1:A:209:LEU:HD11	1:A:310:ARG:CB	2.23	0.58
1:A:397:LEU:HD22	1:A:500:PRO:HG3	1.86	0.58
1:A:448:ARG:CZ	1:A:454:ARG:HG2	2.32	0.58
1:A:478:GLN:NE2	1:A:478:GLN:N	2.51	0.58
1:A:120:TYR:HE1	1:A:127:GLY:O	1.87	0.58
1:A:482:ARG:NH1	1:A:494:LEU:H	2.02	0.57
1:A:263:PHE:CE2	1:A:270:PRO:HG3	2.38	0.57
1:A:85:ASP:O	1:A:89:LEU:N	2.37	0.57
1:A:183:ILE:HG13	1:A:183:ILE:O	2.04	0.57
1:A:256:CYS:HB2	1:A:325:HIS:CE1	2.39	0.56
1:A:466:TYR:O	1:A:466:TYR:CD1	2.59	0.56
1:A:482:ARG:NH1	1:A:494:LEU:HD23	2.21	0.56
1:A:213:TYR:CE1	1:A:294:ILE:HD12	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ILE:H	1:A:407:HIS:HE1	1.53	0.55
1:A:462:PHE:HD2	1:A:471:PRO:HG3	1.71	0.55
1:A:243:THR:HG22	1:A:293:ALA:HA	1.89	0.55
1:A:415:ILE:HG13	1:A:480:TYR:OH	2.06	0.55
1:A:124:THR:HB	1:A:126:HIS:CE1	2.42	0.55
1:A:32:ASP:HA	1:A:139:THR:HG22	1.89	0.55
1:A:420:SER:N	1:A:489:LYS:O	2.39	0.55
1:A:487:ASN:HD22	1:A:488:ALA:N	2.05	0.55
1:A:5:VAL:HG13	1:A:6:PRO:HD2	1.89	0.55
1:A:412:ASP:HB2	1:A:499:ARG:HG2	1.89	0.55
1:A:66:ARG:NH1	1:A:109:LYS:HA	2.22	0.55
1:A:220:LYS:HG3	1:A:225:HIS:NE2	2.22	0.55
1:A:495:ARG:HG3	1:A:495:ARG:HH11	1.72	0.55
1:A:469:ALA:O	1:A:471:PRO:N	2.40	0.54
1:A:209:LEU:CD1	1:A:310:ARG:HB2	2.26	0.54
1:A:448:ARG:NH2	1:A:454:ARG:HG2	2.23	0.54
1:A:468:GLY:O	1:A:470:THR:N	2.40	0.54
1:A:179:MET:HE3	1:A:183:ILE:HA	1.88	0.54
1:A:33:ILE:HD11	1:A:140:LEU:HD13	1.90	0.54
1:A:501:LYS:O	1:A:502:SER:HB2	2.07	0.54
1:A:376:ILE:O	1:A:478:GLN:NE2	2.41	0.54
1:A:400:LEU:O	1:A:404:THR:HB	2.07	0.53
1:A:363:LEU:HD12	1:A:486:VAL:HG11	1.89	0.53
1:A:4:VAL:O	1:A:4:VAL:HG23	2.09	0.53
1:A:33:ILE:O	1:A:37:ILE:HG13	2.09	0.53
1:A:213:TYR:HA	1:A:240:TRP:CZ2	2.44	0.53
1:A:459:ILE:O	1:A:475:LEU:HD21	2.09	0.53
1:A:60:VAL:HG22	1:A:116:TRP:HB3	1.90	0.53
1:A:83:ARG:NH2	1:A:96:SER:OG	2.42	0.52
1:A:487:ASN:ND2	1:A:489:LYS:HG2	2.24	0.52
1:A:419:ARG:HA	1:A:489:LYS:O	2.09	0.52
1:A:476:GLY:O	1:A:477:LYS:C	2.47	0.52
1:A:487:ASN:ND2	1:A:488:ALA:N	2.57	0.52
1:A:104:LYS:HB3	1:A:114:HIS:CD2	2.44	0.52
1:A:83:ARG:HB2	1:A:99:PHE:CE2	2.45	0.52
1:A:98:MET:SD	1:A:221:HIS:HE1	2.33	0.51
1:A:194:TYR:CE1	1:A:334:HIS:HB2	2.45	0.51
1:A:236:ARG:O	1:A:236:ARG:HD3	2.10	0.51
1:A:376:ILE:O	1:A:477:LYS:HA	2.11	0.51
1:A:11:CYS:HG	1:A:37:ILE:HG12	1.75	0.51
1:A:421:LYS:HD2	1:A:489:LYS:HE2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:GLY:O	1:A:294:ILE:HG12	2.10	0.51
1:A:379:TYR:CD1	1:A:467:ALA:HA	2.46	0.51
1:A:485:ILE:H	1:A:485:ILE:CD1	2.12	0.51
1:A:376:ILE:HB	1:A:478:GLN:NE2	2.26	0.50
1:A:81:TYR:CD2	1:A:136:THR:HG22	2.47	0.50
1:A:112:ASP:C	1:A:114:HIS:N	2.65	0.50
1:A:201:LYS:HD2	1:A:202:LEU:H	1.77	0.50
1:A:485:ILE:HG13	1:A:489:LYS:NZ	2.27	0.50
1:A:491:ILE:HG22	1:A:492:VAL:HG23	1.92	0.50
1:A:84:ILE:HG23	1:A:87:PRO:HG2	1.94	0.50
1:A:402:ALA:HA	1:A:466:TYR:CE2	2.47	0.50
1:A:76:CYS:O	1:A:101:LEU:HA	2.12	0.49
1:A:181:TRP:CD1	1:A:500:PRO:HB2	2.47	0.49
1:A:86:LEU:HA	1:A:89:LEU:HD23	1.93	0.49
1:A:466:TYR:CD1	1:A:466:TYR:C	2.86	0.49
1:A:201:LYS:CD	1:A:202:LEU:H	2.25	0.49
1:A:86:LEU:HB2	1:A:87:PRO:HD3	1.93	0.49
1:A:183:ILE:HD13	1:A:233:VAL:O	2.13	0.49
1:A:336:ASN:OD1	1:A:337:THR:HG23	2.12	0.49
1:A:397:LEU:HD23	1:A:498:LEU:CD1	2.42	0.49
1:A:83:ARG:HH12	1:A:96:SER:HB3	1.78	0.48
1:A:480:TYR:CG	1:A:494:LEU:HD21	2.48	0.48
1:A:485:ILE:O	1:A:489:LYS:CG	2.61	0.48
1:A:272:THR:CG2	1:A:274:ARG:HB3	2.43	0.48
1:A:376:ILE:CD1	1:A:480:TYR:HE2	2.26	0.48
1:A:449:ILE:H	1:A:449:ILE:CD1	2.24	0.48
1:A:59:THR:HA	1:A:116:TRP:O	2.14	0.48
1:A:48:TRP:CZ2	1:A:128:LEU:HG	2.48	0.48
1:A:84:ILE:HG12	1:A:87:PRO:HD3	1.95	0.48
1:A:462:PHE:CE1	1:A:463:LEU:CD1	2.97	0.48
1:A:83:ARG:NH1	1:A:96:SER:HB3	2.29	0.48
1:A:466:TYR:HD1	1:A:466:TYR:C	2.17	0.48
1:A:435:ASN:CB	1:A:477:LYS:HE3	2.43	0.48
1:A:31:PHE:HB3	1:A:140:LEU:HB2	1.96	0.48
1:A:93:CYS:O	1:A:97:GLU:HG2	2.14	0.48
1:A:113:VAL:O	1:A:115:GLU:N	2.47	0.48
1:A:461:ILE:HG22	1:A:474:ALA:HA	1.96	0.47
1:A:92:GLU:HB2	1:A:96:SER:OG	2.13	0.47
1:A:272:THR:HB	1:A:275:GLN:HG3	1.96	0.47
1:A:415:ILE:HG23	1:A:494:LEU:HB2	1.96	0.47
1:A:499:ARG:HG3	1:A:499:ARG:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:THR:HG22	1:A:141:TYR:CD1	2.50	0.47
1:A:40:TYR:CG	1:A:41:GLY:N	2.83	0.47
1:A:272:THR:HG22	1:A:274:ARG:HB3	1.95	0.47
1:A:373:ASN:OD1	1:A:481:VAL:HA	2.14	0.47
1:A:485:ILE:HG12	1:A:485:ILE:O	2.15	0.47
1:A:84:ILE:CG2	1:A:87:PRO:HG2	2.45	0.47
1:A:157:GLN:HG3	1:A:158:CYS:N	2.28	0.47
1:A:90:GLY:O	1:A:91:ASN:O	2.32	0.47
1:A:376:ILE:HD12	1:A:480:TYR:HE2	1.80	0.47
1:A:274:ARG:NH1	1:A:278:TRP:NE1	2.63	0.47
1:A:77:THR:HB	1:A:101:LEU:HD22	1.95	0.46
1:A:461:ILE:HD11	1:A:465:SER:N	2.29	0.46
1:A:213:TYR:HD1	1:A:240:TRP:CZ2	2.34	0.46
1:A:78:PHE:HB3	1:A:100:GLU:HG3	1.97	0.46
1:A:495:ARG:HG3	1:A:495:ARG:NH1	2.30	0.46
1:A:471:PRO:HG2	1:A:473:GLY:CA	2.44	0.46
1:A:88:ALA:CA	1:A:223:LYS:HE2	2.44	0.46
1:A:359:THR:HG23	1:A:391:THR:HB	1.97	0.46
1:A:363:LEU:HD12	1:A:486:VAL:CG1	2.46	0.46
1:A:417:TRP:CZ2	1:A:452:LEU:HA	2.50	0.46
1:A:83:ARG:CZ	1:A:96:SER:OG	2.63	0.46
1:A:219:VAL:HG12	1:A:220:LYS:N	2.30	0.46
1:A:270:PRO:O	1:A:272:THR:N	2.49	0.46
1:A:439:TRP:HH2	1:A:443:TRP:HZ3	1.64	0.46
1:A:189:PHE:HB3	1:A:338:TRP:CD1	2.50	0.46
1:A:357:TRP:HB2	1:A:498:LEU:HG	1.98	0.45
1:A:461:ILE:HG21	1:A:469:ALA:HB2	1.98	0.45
1:A:482:ARG:NH2	1:A:494:LEU:CG	2.70	0.45
1:A:484:SER:O	1:A:486:VAL:N	2.48	0.45
1:A:48:TRP:HA	1:A:48:TRP:CE3	2.52	0.45
1:A:189:PHE:HB3	1:A:338:TRP:NE1	2.31	0.45
1:A:211:ILE:HG12	1:A:306:GLU:HG3	1.99	0.45
1:A:449:ILE:N	1:A:449:ILE:CD1	2.74	0.45
1:A:492:VAL:C	1:A:493:ALA:O	2.54	0.45
1:A:78:PHE:HB3	1:A:100:GLU:HB2	1.99	0.45
1:A:273:LEU:HD22	1:A:277:LEU:HG	1.98	0.45
1:A:482:ARG:HH22	1:A:494:LEU:H	1.64	0.45
1:A:485:ILE:CG1	1:A:489:LYS:HZ2	2.30	0.45
1:A:83:ARG:CD	1:A:99:PHE:HE2	2.28	0.45
1:A:262:ILE:HG23	1:A:311:LEU:HD11	1.98	0.45
1:A:419:ARG:HH21	1:A:484:SER:CB	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:ASN:HD21	1:A:489:LYS:NZ	2.15	0.45
1:A:439:TRP:HA	1:A:439:TRP:HE3	1.81	0.45
1:A:439:TRP:CH2	1:A:443:TRP:HZ3	2.35	0.45
1:A:202:LEU:HD23	1:A:319:PRO:N	2.32	0.44
1:A:269:ALA:O	1:A:271:PRO:CD	2.65	0.44
1:A:421:LYS:HD2	1:A:489:LYS:CD	2.47	0.44
1:A:112:ASP:C	1:A:114:HIS:H	2.20	0.44
1:A:442:TYR:O	1:A:443:TRP:CB	2.63	0.44
1:A:482:ARG:HH12	1:A:494:LEU:N	2.12	0.44
1:A:110:ASP:HB2	1:A:113:VAL:CG2	2.47	0.44
1:A:397:LEU:HD22	1:A:500:PRO:CG	2.46	0.44
1:A:112:ASP:O	1:A:114:HIS:N	2.50	0.44
1:A:412:ASP:HB2	1:A:499:ARG:HD3	1.99	0.44
1:A:48:TRP:HA	1:A:48:TRP:HE3	1.82	0.44
1:A:25:GLY:O	1:A:91:ASN:HA	2.18	0.44
1:A:104:LYS:HB3	1:A:114:HIS:HD2	1.82	0.44
1:A:181:TRP:O	1:A:181:TRP:CD2	2.70	0.44
1:A:213:TYR:HA	1:A:240:TRP:HZ2	1.82	0.44
1:A:260:PHE:CD1	1:A:260:PHE:N	2.86	0.44
1:A:421:LYS:CE	1:A:489:LYS:HE2	2.48	0.44
1:A:469:ALA:O	1:A:471:PRO:CD	2.66	0.44
1:A:469:ALA:O	1:A:471:PRO:HD2	2.18	0.44
1:A:84:ILE:HD11	1:A:86:LEU:HD23	1.99	0.43
1:A:363:LEU:HD13	1:A:374:PHE:HE1	1.82	0.43
1:A:452:LEU:HD12	1:A:452:LEU:H	1.82	0.43
1:A:487:ASN:HD21	1:A:489:LYS:HZ2	1.67	0.43
1:A:83:ARG:NH1	1:A:96:SER:CB	2.81	0.43
1:A:365:PRO:HB2	1:A:370:GLY:C	2.39	0.43
1:A:448:ARG:HG2	1:A:448:ARG:HH11	1.84	0.43
1:A:449:ILE:O	1:A:450:TYR:CD1	2.71	0.43
1:A:469:ALA:HB3	1:A:474:ALA:CB	2.48	0.43
1:A:101:LEU:O	1:A:194:TYR:HE2	2.02	0.43
1:A:179:MET:CE	1:A:183:ILE:HA	2.49	0.43
1:A:373:ASN:ND2	1:A:481:VAL:HG22	2.34	0.43
1:A:104:LYS:HD3	1:A:114:HIS:HB3	2.00	0.43
1:A:266:GLU:HG3	1:A:309:GLY:H	1.84	0.43
1:A:209:LEU:HD21	1:A:310:ARG:HG3	2.01	0.42
1:A:106:PHE:CD1	1:A:106:PHE:N	2.87	0.42
1:A:219:VAL:O	1:A:225:HIS:HA	2.20	0.42
1:A:380:ILE:H	1:A:407:HIS:CE1	2.36	0.42
1:A:417:TRP:HB3	1:A:494:LEU:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ASN:O	1:A:121:GLY:N	2.52	0.42
1:A:465:SER:OG	1:A:466:TYR:N	2.51	0.42
1:A:482:ARG:NH2	1:A:494:LEU:H	2.17	0.42
1:A:82:LYS:HD3	1:A:510:ALA:O	2.20	0.42
1:A:220:LYS:HA	1:A:225:HIS:HA	2.00	0.42
1:A:375:ASP:O	1:A:377:PRO:HD3	2.19	0.42
1:A:101:LEU:HD12	1:A:103:THR:HG23	2.02	0.42
1:A:188:THR:CG2	1:A:339:ARG:HG3	2.42	0.42
1:A:338:TRP:CZ3	1:A:340:PRO:HA	2.54	0.42
1:A:397:LEU:CD2	1:A:498:LEU:HD13	2.49	0.42
1:A:35:GLN:OE1	1:A:35:GLN:HA	2.19	0.42
1:A:191:ILE:H	1:A:191:ILE:HG12	1.69	0.42
1:A:448:ARG:HH11	1:A:448:ARG:CG	2.31	0.42
1:A:431:SER:OG	1:A:483:ILE:HD11	2.19	0.42
1:A:446:GLN:HE22	1:A:454:ARG:NH2	2.14	0.42
1:A:185:LEU:HD23	1:A:185:LEU:HA	1.74	0.42
1:A:227:ILE:HG13	1:A:513:PHE:HE1	1.85	0.42
1:A:414:CYS:HB2	1:A:497:CYS:CB	2.49	0.41
1:A:485:ILE:CG1	1:A:489:LYS:HG3	2.41	0.41
1:A:106:PHE:N	1:A:106:PHE:HD1	2.18	0.41
1:A:213:TYR:HE2	1:A:310:ARG:C	2.23	0.41
1:A:273:LEU:HD13	1:A:277:LEU:CD1	2.50	0.41
1:A:415:ILE:CD1	1:A:496:VAL:HG22	2.50	0.41
1:A:469:ALA:HB3	1:A:474:ALA:HB1	2.02	0.41
1:A:212:SER:HB3	1:A:213:TYR:CZ	2.55	0.41
1:A:467:ALA:O	1:A:468:GLY:C	2.59	0.41
1:A:475:LEU:HD23	1:A:475:LEU:N	2.35	0.41
1:A:213:TYR:CE1	1:A:294:ILE:HG23	2.56	0.41
1:A:363:LEU:HD13	1:A:374:PHE:CZ	2.56	0.41
1:A:30:THR:HA	1:A:140:LEU:O	2.21	0.41
1:A:119:ASN:HB3	1:A:122:GLU:HB2	2.03	0.41
1:A:178:THR:O	1:A:179:MET:HG2	2.21	0.41
1:A:181:TRP:HB3	1:A:182:PRO:HD3	2.03	0.41
1:A:477:LYS:O	1:A:477:LYS:HG3	2.21	0.41
1:A:482:ARG:HH22	1:A:494:LEU:N	2.19	0.41
1:A:100:GLU:O	1:A:101:LEU:HB2	2.19	0.40
1:A:212:SER:HA	1:A:215:PHE:HE1	1.85	0.40
1:A:48:TRP:HZ3	1:A:54:VAL:HG22	1.86	0.40
1:A:302:ALA:HB3	1:A:305:GLU:O	2.21	0.40
1:A:397:LEU:CD2	1:A:500:PRO:HG3	2.50	0.40
1:A:458:GLU:OE2	1:A:476:GLY:HA3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:ASP:O	1:A:491:ILE:C	2.60	0.40
1:A:23:LYS:HA	1:A:23:LYS:HD3	1.77	0.40
1:A:93:CYS:CB	1:A:94:PRO:HD3	2.43	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	511/513 (100%)	397 (78%)	70 (14%)	44 (9%)	1 9

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	LEU
1	A	91	ASN
1	A	93	CYS
1	A	109	LYS
1	A	203	ASP
1	A	211	ILE
1	A	377	PRO
1	A	421	LYS
1	A	461	ILE
1	A	469	ALA
1	A	470	THR
1	A	487	ASN
1	A	493	ALA
1	A	502	SER
1	A	24	LYS
1	A	25	GLY
1	A	41	GLY
1	A	112	ASP

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Mol	Chain	Res	Type
1	A	207	SER
1	A	214	ASN
1	A	439	TRP
1	A	443	TRP
1	A	110	ASP
1	A	204	GLY
1	A	269	ALA
1	A	318	GLY
1	A	342	SER
1	A	471	PRO
1	A	475	LEU
1	A	477	LYS
1	A	491	ILE
1	A	102	PRO
1	A	196	GLU
1	A	462	PHE
1	A	86	LEU
1	A	271	PRO
1	A	378	GLY
1	A	453	ARG
1	A	270	PRO
1	A	438	ASP
1	A	216	GLY
1	A	481	VAL
1	A	468	GLY
1	A	464	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	431/431 (100%)	371 (86%)	60 (14%)	3 20

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	TRP
1	A	49	CYS
1	A	53	ILE
1	A	59	THR
1	A	81	TYR
1	A	86	LEU
1	A	89	LEU
1	A	91	ASN
1	A	98	MET
1	A	101	LEU
1	A	107	MET
1	A	110	ASP
1	A	122	GLU
1	A	148	ASN
1	A	149	GLN
1	A	157	GLN
1	A	180	THR
1	A	183	ILE
1	A	202	LEU
1	A	209	LEU
1	A	228	SER
1	A	236	ARG
1	A	272	THR
1	A	273	LEU
1	A	274	ARG
1	A	278	TRP
1	A	320	ILE
1	A	328	SER
1	A	339	ARG
1	A	354	LEU
1	A	356	ASN
1	A	359	THR
1	A	360	LEU
1	A	361	THR
1	A	366	ASP
1	A	369	THR
1	A	395	ASN
1	A	404	THR
1	A	419	ARG
1	A	437	ARG
1	A	438	ASP
1	A	439	TRP
1	A	443	TRP

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Mol	Chain	Res	Type
1	A	444	GLN
1	A	448	ARG
1	A	449	ILE
1	A	452	LEU
1	A	460	PRO
1	A	461	ILE
1	A	466	TYR
1	A	470	THR
1	A	478	GLN
1	A	479	ASN
1	A	485	ILE
1	A	487	ASN
1	A	490	ASP
1	A	495	ARG
1	A	497	CYS
1	A	498	LEU
1	A	511	THR

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

Mol	Chain	Res	Type
1	A	44	HIS
1	A	55	ASN
1	A	91	ASN
1	A	149	GLN
1	A	221	HIS
1	A	285	HIS
1	A	299	HIS
1	A	325	HIS
1	A	356	ASN
1	A	407	HIS
1	A	435	ASN
1	A	446	GLN
1	A	478	GLN
1	A	487	ASN

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	513/513 (100%)	-1.01	0	100	100	15, 15, 15, 15	0

There are no RSRZ outliers to report.

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.