Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 01:09 AM EDT

PDB ID	:	2QJ1
Title	:	Crystal structure of infectious bursal disease virus VP1 polymerase incubated with an oligopeptide mimicking the VP3 C-terminus
Authors	:	Garriga, D.; Navarro, A.; Querol-Audi, J.; Abaitua, F.; Rodriguez, J.F.; Verdaguer, N.
Deposited on	:	2007-07-06
Resolution	:	3.48 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:

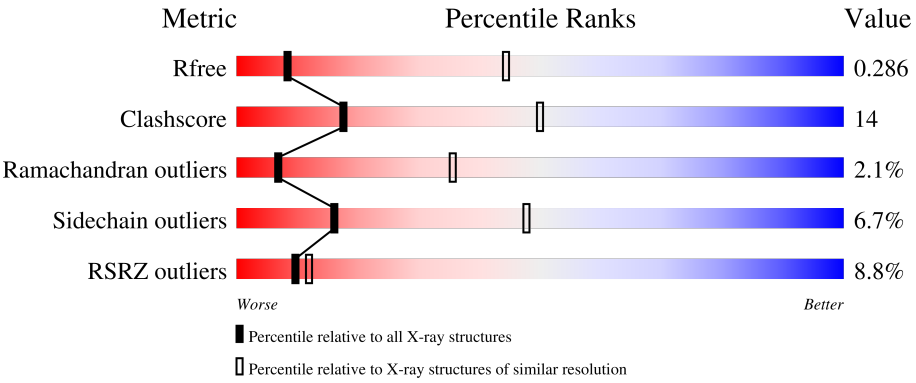
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.48 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	1379 (3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)

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	852	8% 63% 23% · 10%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5927 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 Infectious bursal disease virus VP1 polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	767	5927	3793	1009	1103	22	14	0	0

There are 8 discrepancies between the modelled and reference sequences:

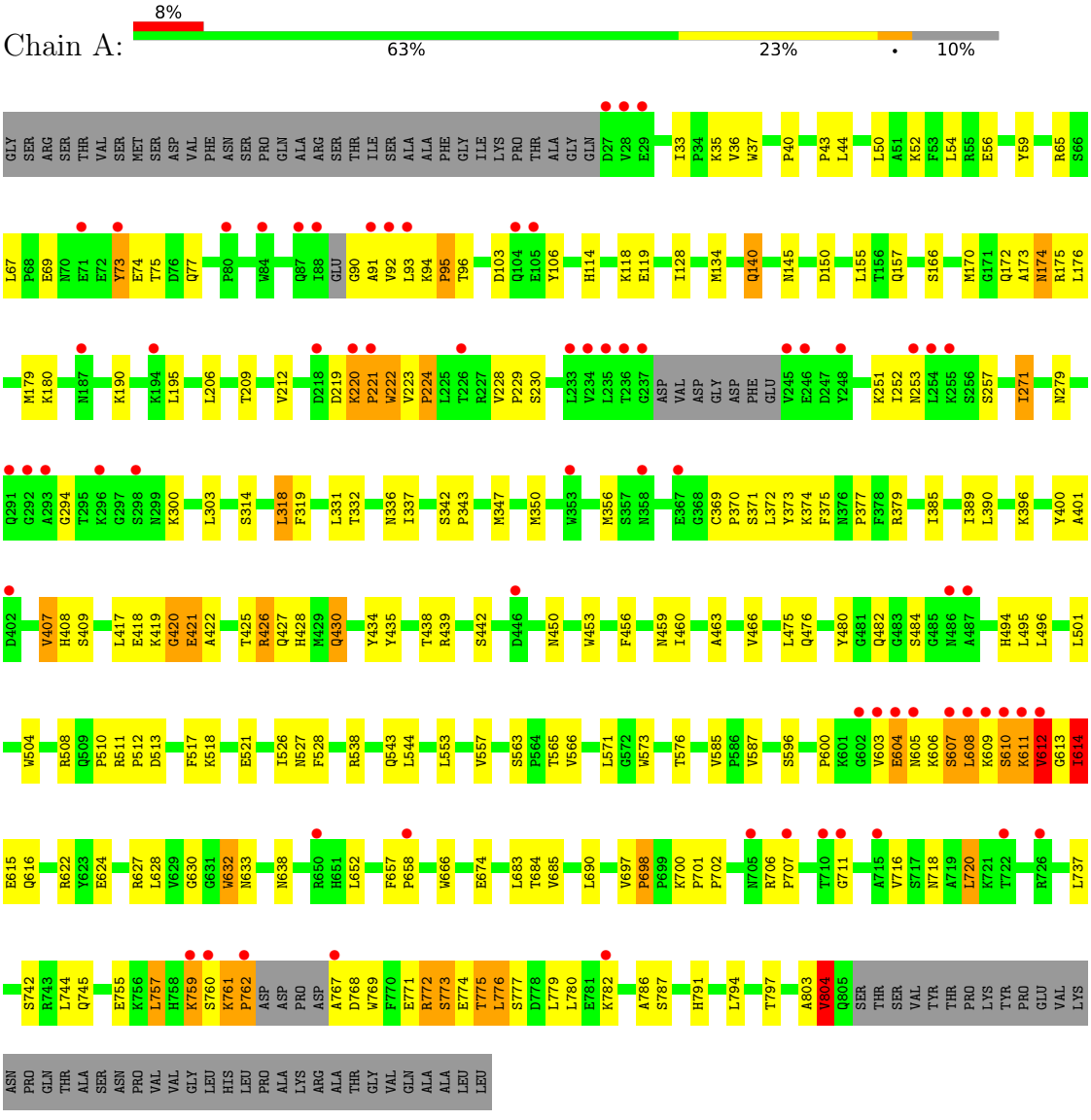
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP Q82629
A	-5	SER	-	expression tag	UNP Q82629
A	-4	ARG	-	expression tag	UNP Q82629
A	-3	SER	-	expression tag	UNP Q82629
A	-2	THR	-	expression tag	UNP Q82629
A	-1	VAL	-	expression tag	UNP Q82629
A	0	SER	-	expression tag	UNP Q82629
A	4	VAL	ILE	SEE REMARK 999	UNP Q82629

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: Infectious bursal disease virus VP1 polymerase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	121.91Å 121.91Å 359.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.98 – 3.48 19.98 – 3.48	Depositor EDS
% Data completeness (in resolution range)	96.5 (19.98-3.48) 96.5 (19.98-3.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.55 (at 3.52Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.241 , 0.281 0.262 , 0.286	Depositor DCC
R_{free} test set	1039 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	84.1	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 67.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	5927	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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	A	0.35	0/6066	0.69	18/8250 (0.2%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	610	SER	CB-CA-C	-14.71	82.16	110.10
1	A	421	GLU	N-CA-CB	12.95	133.90	110.60
1	A	420	GLY	N-CA-C	-11.84	83.51	113.10
1	A	222	TRP	CB-CA-C	-11.68	87.05	110.40
1	A	611	LYS	N-CA-CB	-11.25	90.35	110.60
1	A	612	VAL	N-CA-CB	-10.35	88.73	111.50
1	A	93	LEU	N-CA-CB	-9.69	91.03	110.40
1	A	421	GLU	CB-CA-C	-9.43	91.55	110.40
1	A	611	LYS	N-CA-C	-8.39	88.34	111.00
1	A	767	ALA	N-CA-C	7.96	132.48	111.00
1	A	804	VAL	N-CA-C	-7.82	89.89	111.00
1	A	610	SER	N-CA-C	7.66	131.67	111.00
1	A	611	LYS	CB-CA-C	-7.50	95.41	110.40
1	A	768	ASP	N-CA-C	-7.14	91.71	111.00
1	A	422	ALA	N-CA-CB	6.84	119.67	110.10
1	A	762	PRO	N-CA-CB	5.93	110.42	103.30
1	A	222	TRP	N-CA-C	5.71	126.43	111.00
1	A	604	GLU	N-CA-C	-5.00	97.50	111.00

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	5927	0	5873	161	0
All	All	5927	0	5873	161	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 14.

All (161) 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:92:VAL:O	1:A:271:ILE:HD11	1.17	1.26
1:A:92:VAL:O	1:A:271:ILE:CD1	1.82	1.26
1:A:140:GLN:HE21	1:A:140:GLN:HA	1.24	1.02
1:A:221:PRO:O	1:A:222:TRP:HB2	1.67	0.91
1:A:421:GLU:HG2	1:A:484:SER:HA	1.53	0.90
1:A:611:LYS:O	1:A:657:PHE:CD1	2.24	0.89
1:A:600:PRO:HB3	1:A:622:ARG:HD2	1.55	0.88
1:A:610:SER:H	1:A:614:ILE:HG12	1.40	0.87
1:A:613:GLY:O	1:A:614:ILE:C	2.15	0.85
1:A:230:SER:HB2	1:A:279:ASN:HD21	1.44	0.83
1:A:737:LEU:HD11	1:A:769:TRP:HE1	1.45	0.81
1:A:609:LYS:CB	1:A:614:ILE:HD11	2.10	0.80
1:A:459:ASN:O	1:A:797:THR:HG21	1.82	0.79
1:A:92:VAL:O	1:A:271:ILE:HD13	1.82	0.76
1:A:772:ARG:HA	1:A:775:THR:OG1	1.84	0.76
1:A:611:LYS:O	1:A:657:PHE:HD1	1.65	0.75
1:A:222:TRP:O	1:A:224:PRO:HD3	1.87	0.74
1:A:757:LEU:HD12	1:A:779:LEU:HD12	1.69	0.74
1:A:610:SER:N	1:A:614:ILE:HG12	2.03	0.73
1:A:220:LYS:CB	1:A:221:PRO:CD	2.67	0.72
1:A:737:LEU:HD21	1:A:769:TRP:HZ2	1.55	0.72
1:A:173:ALA:HA	1:A:176:LEU:HD12	1.73	0.70
1:A:611:LYS:O	1:A:657:PHE:CE1	2.44	0.70
1:A:69:GLU:HG2	1:A:106:TYR:HD1	1.56	0.70
1:A:75:THR:OG1	1:A:94:LYS:O	2.11	0.68
1:A:610:SER:O	1:A:612:VAL:N	2.27	0.68
1:A:303:LEU:HD21	1:A:744:LEU:HD22	1.75	0.67
1:A:511:ARG:HD3	1:A:513:ASP:OD1	1.95	0.66
1:A:706:ARG:HB2	1:A:707:PRO:HD2	1.77	0.66
1:A:504:TRP:CD1	1:A:510:PRO:HD2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:LYS:C	1:A:420:GLY:O	2.25	0.65
1:A:757:LEU:CD1	1:A:776:LEU:HA	2.27	0.65
1:A:757:LEU:HD13	1:A:776:LEU:HA	1.79	0.64
1:A:611:LYS:CB	1:A:657:PHE:CE1	2.81	0.64
1:A:610:SER:H	1:A:614:ILE:CG1	2.10	0.63
1:A:606:LYS:C	1:A:608:LEU:H	2.01	0.63
1:A:565:THR:HG22	1:A:576:THR:HB	1.80	0.63
1:A:418:GLU:HB2	1:A:527:ASN:HB2	1.81	0.62
1:A:157:GLN:HA	1:A:157:GLN:HE21	1.65	0.61
1:A:172:GLN:HB3	1:A:336:ASN:HD21	1.66	0.61
1:A:140:GLN:HA	1:A:140:GLN:NE2	2.06	0.61
1:A:614:ILE:HG22	1:A:615:GLU:N	2.14	0.60
1:A:425:THR:H	1:A:428:HIS:HD2	1.48	0.60
1:A:761:LYS:O	1:A:762:PRO:CB	2.50	0.59
1:A:737:LEU:HD11	1:A:769:TRP:NE1	2.15	0.58
1:A:373:TYR:HA	1:A:400:TYR:CE2	2.38	0.58
1:A:33:ILE:HG23	1:A:128:ILE:HD12	1.86	0.57
1:A:616:GLN:HB2	1:A:652:LEU:HD21	1.87	0.57
1:A:772:ARG:CA	1:A:775:THR:OG1	2.51	0.56
1:A:170:MET:O	1:A:174:ASN:HB2	2.06	0.56
1:A:220:LYS:CB	1:A:221:PRO:HD3	2.35	0.56
1:A:157:GLN:HA	1:A:157:GLN:NE2	2.21	0.55
1:A:375:PHE:HD2	1:A:571:LEU:HD12	1.72	0.55
1:A:456:PHE:HA	1:A:460:ILE:HB	1.89	0.54
1:A:612:VAL:O	1:A:657:PHE:HB2	2.06	0.54
1:A:606:LYS:O	1:A:608:LEU:N	2.41	0.54
1:A:435:TYR:CE2	1:A:439:ARG:HD2	2.42	0.54
1:A:209:THR:O	1:A:371:SER:HB2	2.08	0.54
1:A:420:GLY:O	1:A:421:GLU:OE1	2.25	0.53
1:A:90:GLY:N	1:A:251:LYS:HE3	2.23	0.53
1:A:37:TRP:CZ2	1:A:40:PRO:HD3	2.44	0.53
1:A:613:GLY:O	1:A:616:GLN:N	2.41	0.53
1:A:94:LYS:O	1:A:96:THR:N	2.42	0.52
1:A:609:LYS:O	1:A:610:SER:CB	2.57	0.52
1:A:427:GLN:HA	1:A:430:GLN:HG2	1.91	0.52
1:A:35:LYS:HG2	1:A:36:VAL:N	2.25	0.52
1:A:417:LEU:HD23	1:A:528:PHE:HB3	1.92	0.52
1:A:426:ARG:HD3	1:A:463:ALA:HA	1.91	0.52
1:A:52:LYS:O	1:A:56:GLU:HB2	2.10	0.52
1:A:773:SER:OG	1:A:774:GLU:N	2.43	0.51
1:A:613:GLY:O	1:A:615:GLU:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:GLN:HE21	1:A:140:GLN:CA	2.06	0.51
1:A:426:ARG:HG2	1:A:466:VAL:HB	1.94	0.50
1:A:319:PHE:HB3	1:A:337:ILE:HB	1.93	0.50
1:A:606:LYS:C	1:A:608:LEU:N	2.65	0.50
1:A:170:MET:HG3	1:A:331:LEU:O	2.11	0.50
1:A:221:PRO:O	1:A:222:TRP:CB	2.50	0.50
1:A:627:ARG:HD2	1:A:638:ASN:OD1	2.11	0.50
1:A:742:SER:HA	1:A:787:SER:H	1.77	0.50
1:A:418:GLU:O	1:A:419:LYS:C	2.51	0.49
1:A:521:GLU:HB2	1:A:526:ILE:O	2.12	0.49
1:A:780:LEU:HB3	1:A:786:ALA:HB2	1.95	0.49
1:A:600:PRO:CB	1:A:622:ARG:HD2	2.37	0.49
1:A:408:HIS:CE1	1:A:409:SER:HG	2.31	0.48
1:A:611:LYS:O	1:A:612:VAL:C	2.52	0.48
1:A:180:LYS:HG3	1:A:480:TYR:CZ	2.47	0.48
1:A:43:PRO:HB2	1:A:170:MET:HE2	1.93	0.48
1:A:544:LEU:HD21	1:A:566:VAL:HG23	1.94	0.48
1:A:229:PRO:HG3	1:A:350:MET:CE	2.42	0.48
1:A:624:GLU:HB3	1:A:683:LEU:HD22	1.94	0.48
1:A:518:LYS:O	1:A:521:GLU:HG2	2.14	0.48
1:A:587:VAL:HG22	1:A:632:TRP:CZ2	2.49	0.47
1:A:421:GLU:O	1:A:482:GLN:O	2.33	0.47
1:A:114:HIS:HA	1:A:166:SER:HB2	1.97	0.47
1:A:212:VAL:HG12	1:A:356:MET:HE2	1.96	0.47
1:A:228:VAL:HB	1:A:229:PRO:HD2	1.97	0.47
1:A:553:LEU:HD13	1:A:585:VAL:HG21	1.97	0.47
1:A:771:GLU:O	1:A:775:THR:OG1	2.33	0.47
1:A:65:ARG:H	1:A:476:GLN:HE22	1.63	0.46
1:A:43:PRO:HD2	1:A:170:MET:HB2	1.98	0.46
1:A:94:LYS:O	1:A:95:PRO:C	2.54	0.46
1:A:611:LYS:CB	1:A:657:PHE:HE1	2.29	0.46
1:A:373:TYR:CE2	1:A:374:LYS:HG3	2.51	0.46
1:A:174:ASN:HD22	1:A:332:THR:HA	1.81	0.45
1:A:755:GLU:O	1:A:759:LYS:HG2	2.16	0.45
1:A:50:LEU:HD23	1:A:475:LEU:HD12	1.97	0.45
1:A:803:ALA:O	1:A:804:VAL:C	2.53	0.45
1:A:303:LEU:HD22	1:A:745:GLN:HG2	1.97	0.45
1:A:418:GLU:HB2	1:A:527:ASN:CB	2.46	0.45
1:A:628:LEU:HD13	1:A:685:VAL:HG22	1.99	0.45
1:A:176:LEU:HD11	1:A:318:LEU:HD11	1.99	0.45
1:A:74:GLU:HA	1:A:96:THR:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:SER:HB2	1:A:279:ASN:ND2	2.23	0.44
1:A:206:LEU:HD11	1:A:495:LEU:HD12	2.00	0.44
1:A:372:LEU:O	1:A:375:PHE:HB3	2.17	0.44
1:A:434:TYR:CZ	1:A:438:THR:HG21	2.53	0.44
1:A:91:ALA:O	1:A:92:VAL:C	2.55	0.44
1:A:512:PRO:HA	1:A:517:PHE:CG	2.53	0.44
1:A:212:VAL:HG12	1:A:356:MET:CE	2.48	0.43
1:A:604:GLU:O	1:A:605:ASN:C	2.56	0.43
1:A:134:MET:SD	1:A:155:LEU:HD22	2.58	0.43
1:A:701:PRO:HA	1:A:702:PRO:HD3	1.88	0.43
1:A:176:LEU:HD21	1:A:318:LEU:HD11	2.01	0.43
1:A:419:LYS:O	1:A:420:GLY:C	2.56	0.43
1:A:803:ALA:C	1:A:804:VAL:O	2.50	0.43
1:A:610:SER:HA	1:A:614:ILE:HG12	2.01	0.43
1:A:716:VAL:O	1:A:720:LEU:HB2	2.18	0.43
1:A:175:ARG:O	1:A:179:MET:HG3	2.19	0.42
1:A:613:GLY:HA3	1:A:652:LEU:CD2	2.49	0.42
1:A:737:LEU:CD2	1:A:769:TRP:HZ2	2.29	0.42
1:A:342:SER:OG	1:A:343:PRO:HD3	2.20	0.42
1:A:73:TYR:CE1	1:A:77:GLN:HG2	2.55	0.42
1:A:190:LYS:HD3	1:A:195:LEU:HD21	2.00	0.42
1:A:369:CYS:HA	1:A:370:PRO:HD3	1.91	0.42
1:A:563:SER:HB3	1:A:633:ASN:OD1	2.20	0.42
1:A:627:ARG:HB3	1:A:685:VAL:HG11	2.00	0.42
1:A:390:LEU:HA	1:A:538:ARG:HG2	2.00	0.42
1:A:396:LYS:HG3	1:A:407:VAL:HG13	2.02	0.42
1:A:377:PRO:HG3	1:A:573:TRP:CE2	2.54	0.42
1:A:54:LEU:HB3	1:A:59:TYR:HB3	2.02	0.42
1:A:347:MET:HA	1:A:350:MET:HE3	2.01	0.42
1:A:229:PRO:HG3	1:A:350:MET:HE1	2.01	0.41
1:A:401:ALA:H	1:A:494:HIS:CD2	2.38	0.41
1:A:385:ILE:O	1:A:389:ILE:HG13	2.20	0.41
1:A:40:PRO:HB2	1:A:331:LEU:HD21	2.01	0.41
1:A:118:LYS:HG3	1:A:119:GLU:N	2.35	0.41
1:A:425:THR:H	1:A:428:HIS:CD2	2.34	0.41
1:A:611:LYS:C	1:A:657:PHE:HD1	2.22	0.41
1:A:179:MET:HG2	1:A:419:LYS:HG2	2.02	0.41
1:A:438:THR:O	1:A:442:SER:HB2	2.20	0.41
1:A:607:SER:O	1:A:608:LEU:C	2.59	0.41
1:A:779:LEU:HD23	1:A:782:LYS:HD3	2.01	0.41
1:A:657:PHE:HA	1:A:658:PRO:HD3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:VAL:O	1:A:604:GLU:C	2.57	0.41
1:A:697:VAL:HA	1:A:698:PRO:HD2	1.81	0.41
1:A:610:SER:O	1:A:611:LYS:C	2.58	0.41
1:A:666:TRP:CE2	1:A:683:LEU:HG	2.56	0.40
1:A:44:LEU:HD12	1:A:170:MET:HA	2.03	0.40
1:A:373:TYR:HA	1:A:400:TYR:HE2	1.82	0.40
1:A:450:ASN:HD22	1:A:453:TRP:HD1	1.69	0.40
1:A:607:SER:O	1:A:609:LYS:N	2.54	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	759/852 (89%)	675 (89%)	68 (9%)	16 (2%)	7 35

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	ASP
1	A	220	LYS
1	A	221	PRO
1	A	612	VAL
1	A	614	ILE
1	A	224	PRO
1	A	804	VAL
1	A	607	SER
1	A	630	GLY
1	A	761	LYS
1	A	608	LEU
1	A	95	PRO
1	A	632	TRP

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Mol	Chain	Res	Type
1	A	711	GLY
1	A	698	PRO
1	A	294	GLY

5.3.2 Protein sidechains

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	627/730 (86%)	585 (93%)	42 (7%)	16 48

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	73	TYR
1	A	103	ASP
1	A	140	GLN
1	A	145	ASN
1	A	150	ASP
1	A	174	ASN
1	A	223	VAL
1	A	252	ILE
1	A	253	ASN
1	A	257	SER
1	A	271	ILE
1	A	300	LYS
1	A	314	SER
1	A	318	LEU
1	A	379	ARG
1	A	407	VAL
1	A	426	ARG
1	A	430	GLN
1	A	496	LEU
1	A	501	LEU
1	A	508	ARG
1	A	543	GLN

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Mol	Chain	Res	Type
1	A	557	VAL
1	A	596	SER
1	A	614	ILE
1	A	674	GLU
1	A	684	THR
1	A	690	LEU
1	A	700	LYS
1	A	718	ASN
1	A	720	LEU
1	A	757	LEU
1	A	759	LYS
1	A	760	SER
1	A	772	ARG
1	A	773	SER
1	A	775	THR
1	A	776	LEU
1	A	777	SER
1	A	791	HIS
1	A	794	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	GLN
1	A	145	ASN
1	A	157	GLN
1	A	172	GLN
1	A	204	GLN
1	A	279	ASN
1	A	299	ASN
1	A	336	ASN
1	A	345	HIS
1	A	403	ASN
1	A	428	HIS
1	A	430	GLN
1	A	450	ASN
1	A	451	GLN
1	A	476	GLN
1	A	494	HIS
1	A	503	GLN
1	A	543	GLN
1	A	549	GLN

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Mol	Chain	Res	Type
1	A	745	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 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	A	764/852 (89%)	0.43	67 (8%)	10	12	20, 74, 103, 123	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	245	VAL	7.0
1	A	88	ILE	6.7
1	A	234	VAL	6.4
1	A	27	ASP	5.5
1	A	87	GLN	5.4
1	A	767	ALA	5.3
1	A	610	SER	5.3
1	A	612	VAL	5.1
1	A	235	LEU	5.1
1	A	246	GLU	4.9
1	A	28	VAL	4.6
1	A	218	ASP	4.4
1	A	710	THR	4.2
1	A	603	VAL	4.2
1	A	611	LYS	4.2
1	A	604	GLU	4.1
1	A	80	PRO	4.0
1	A	707	PRO	4.0
1	A	605	ASN	4.0
1	A	233	LEU	4.0
1	A	254	LEU	4.0
1	A	609	LYS	3.9
1	A	782	LYS	3.8
1	A	486	ASN	3.7
1	A	358	ASN	3.6
1	A	29	GLU	3.6
1	A	71	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	759	LYS	3.4
1	A	237	GLY	3.4
1	A	220	LYS	3.3
1	A	353	TRP	3.3
1	A	93	LEU	3.3
1	A	236	THR	3.3
1	A	446	ASP	3.3
1	A	255	LYS	3.2
1	A	367	GLU	3.2
1	A	705	ASN	3.2
1	A	608	LEU	3.2
1	A	762	PRO	3.0
1	A	760	SER	2.9
1	A	92	VAL	2.9
1	A	221	PRO	2.9
1	A	84	TRP	2.9
1	A	91	ALA	2.8
1	A	296	LYS	2.8
1	A	187	ASN	2.7
1	A	292	GLY	2.7
1	A	607	SER	2.6
1	A	650	ARG	2.6
1	A	298	SER	2.5
1	A	104	GLN	2.5
1	A	658	PRO	2.5
1	A	194	LYS	2.5
1	A	73	TYR	2.4
1	A	248	TYR	2.4
1	A	291	GLN	2.3
1	A	105	GLU	2.3
1	A	226	THR	2.3
1	A	726	ARG	2.3
1	A	602	GLY	2.2
1	A	487	ALA	2.2
1	A	402	ASP	2.2
1	A	722	THR	2.2
1	A	715	ALA	2.1
1	A	253	ASN	2.1
1	A	293	ALA	2.1
1	A	711	GLY	2.1

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.