



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:55 am BST

PDB ID : 1Z14
Title : Structural Determinants of Tissue Tropism and In Vivo Pathogenicity for the Parvovirus Minute Virus of Mice
Authors : Kontou, M.; Govindasamy, L.; Nam, H.J.; Bryant, N.; Llamas-Saiz, A.L.; Foces-Foces, C.; Hernando, E.; Rubio, M.P.; McKenna, R.; Almendral, J.M.; Agbandje-McKenna, M.
Deposited on : 2005-03-03
Resolution : 3.25 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

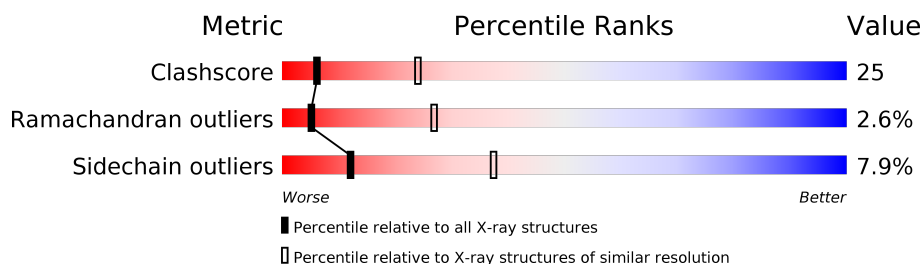
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)

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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	549	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4438 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 VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	0	0
			4317	2724	746	828	19			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	276	PRO	SER	SEE REMARK 999	UNP Q84367

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	121	Total	O	0	0
			121	121		

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

- Molecule 1: VP2



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	448.70 Å 416.50 Å 306.10 Å 90.00° 95.90° 90.00°	Depositor
Resolution (Å)	20.00 – 3.25	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.25)	Depositor
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.298 , 0.306	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4438	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

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	0.69	4/4441 (0.1%)	0.82	9/6073 (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
1	A	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	350	ALA	CA-CB	-11.50	1.28	1.52
1	A	347	ALA	CA-CB	-10.04	1.31	1.52
1	A	464	PRO	N-CD	-8.16	1.36	1.47
1	A	364	GLN	N-CA	7.99	1.62	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	GLU	O-C-N	-11.46	104.36	122.70
1	A	364	GLN	N-CA-C	-9.53	85.27	111.00
1	A	226	GLU	CA-C-N	8.26	135.37	117.20
1	A	226	GLU	C-N-CA	-7.21	103.66	121.70
1	A	349	ARG	NE-CZ-NH1	-6.20	117.20	120.30
1	A	351	GLY	N-CA-C	-6.18	97.64	113.10
1	A	349	ARG	NE-CZ-NH2	5.80	123.20	120.30
1	A	226	GLU	CB-CG-CD	5.31	128.53	114.20
1	A	436	GLY	N-CA-C	-5.09	100.39	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	348	SER	Peptide
1	A	416	SER	Peptide

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	4317	0	4123	207	0
2	A	121	0	0	0	0
All	All	4438	0	4123	207	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 25.

All (207) 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:421:VAL:HB	1:A:422:PRO:HD3	1.25	1.13
1:A:284:GLN:NE2	1:A:586:THR:H	1.60	0.99
1:A:206:THR:HG22	1:A:207:ILE:H	1.28	0.98
1:A:284:GLN:HE21	1:A:586:THR:H	0.94	0.93
1:A:295:LEU:HD12	1:A:295:LEU:H	1.30	0.92
1:A:284:GLN:HE22	1:A:587:TYR:H	1.17	0.92
1:A:463:TYR:HB3	1:A:464:PRO:HD3	1.52	0.92
1:A:206:THR:HG22	1:A:207:ILE:N	1.85	0.90
1:A:49:ASN:HD22	1:A:68:THR:H	1.17	0.90
1:A:433:ASN:N	1:A:433:ASN:HD22	1.66	0.90
1:A:421:VAL:CB	1:A:422:PRO:HD3	2.02	0.89
1:A:417:ALA:HB3	1:A:418:PRO:CD	2.09	0.82
1:A:286:ASN:HD21	1:A:335:GLN:HA	1.44	0.80
1:A:49:ASN:ND2	1:A:68:THR:H	1.79	0.80
1:A:286:ASN:HD22	1:A:336:VAL:H	1.30	0.80
1:A:206:THR:CG2	1:A:207:ILE:H	1.96	0.78
1:A:284:GLN:HE21	1:A:586:THR:N	1.78	0.78
1:A:421:VAL:HB	1:A:422:PRO:CD	2.09	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:THR:HG23	1:A:584:ARG:HH11	1.50	0.77
1:A:285:THR:H	1:A:288:GLN:NE2	1.84	0.76
1:A:367:ASP:HB3	1:A:370:ALA:HB3	1.66	0.76
1:A:342:HIS:H	1:A:342:HIS:CD2	2.02	0.76
1:A:256:ILE:HD12	1:A:256:ILE:N	2.02	0.75
1:A:69:ARG:HH21	1:A:202:PRO:HG3	1.52	0.74
1:A:551:ALA:HB1	1:A:561:VAL:HG12	1.69	0.74
1:A:295:LEU:HD12	1:A:295:LEU:N	2.03	0.74
1:A:463:TYR:CB	1:A:464:PRO:HD3	2.17	0.73
1:A:219:ARG:HD3	1:A:220:ASP:N	2.04	0.73
1:A:69:ARG:NH2	1:A:202:PRO:HG3	2.04	0.72
1:A:281:HIS:HD2	1:A:580:ARG:O	1.71	0.72
1:A:461:PRO:HD2	1:A:579:THR:HG21	1.71	0.72
1:A:417:ALA:CB	1:A:418:PRO:CD	2.68	0.71
1:A:433:ASN:N	1:A:433:ASN:ND2	2.37	0.71
1:A:342:HIS:HD2	1:A:445:ASN:HA	1.56	0.71
1:A:578:ILE:HD12	1:A:578:ILE:H	1.56	0.70
1:A:115:ASP:O	1:A:198:LEU:HD13	1.91	0.70
1:A:380:LYS:HA	1:A:384:GLU:HB3	1.75	0.69
1:A:113:LEU:HD23	1:A:209:SER:O	1.95	0.67
1:A:286:ASN:ND2	1:A:336:VAL:H	1.91	0.67
1:A:500:ARG:HD3	1:A:501:LEU:O	1.93	0.67
1:A:348:SER:O	1:A:350:ALA:N	2.28	0.65
1:A:433:ASN:HD22	1:A:433:ASN:H	1.44	0.65
1:A:342:HIS:CD2	1:A:445:ASN:HA	2.31	0.65
1:A:207:ILE:O	1:A:207:ILE:HD12	1.97	0.65
1:A:284:GLN:NE2	1:A:586:THR:N	2.40	0.65
1:A:295:LEU:H	1:A:295:LEU:CD1	2.05	0.65
1:A:150:VAL:HG21	1:A:259:LEU:HD13	1.78	0.65
1:A:417:ALA:CB	1:A:418:PRO:HD3	2.28	0.64
1:A:45:GLY:HA3	1:A:148:PHE:CD1	2.33	0.64
1:A:284:GLN:NE2	1:A:587:TYR:H	1.93	0.64
1:A:462:VAL:HG23	1:A:466:GLY:HA3	1.80	0.63
1:A:443:PHE:CD2	1:A:444:SER:N	2.67	0.62
1:A:135:MET:SD	1:A:537:LEU:HD23	2.39	0.61
1:A:281:HIS:CE1	1:A:583:ALA:HB2	2.36	0.61
1:A:433:ASN:ND2	1:A:433:ASN:H	1.99	0.61
1:A:285:THR:HG22	1:A:404:GLY:HA2	1.83	0.61
1:A:286:ASN:ND2	1:A:335:GLN:HA	2.15	0.60
1:A:190:PRO:O	1:A:193:ASN:HB2	2.01	0.60
1:A:330:ARG:HD3	1:A:332:ARG:NH1	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:ALA:HB3	1:A:418:PRO:HD2	1.83	0.59
1:A:417:ALA:HB3	1:A:418:PRO:HD3	1.83	0.59
1:A:218:ASP:OD1	1:A:349:ARG:NH1	2.36	0.59
1:A:178:VAL:HG12	1:A:179:ALA:N	2.18	0.59
1:A:85:ARG:HD2	1:A:237:MET:HG2	1.85	0.58
1:A:256:ILE:HD12	1:A:256:ILE:H	1.68	0.58
1:A:194:SER:HB2	1:A:196:GLU:HG3	1.84	0.58
1:A:425:LEU:HD13	1:A:425:LEU:C	2.24	0.58
1:A:126:SER:O	1:A:129:GLN:HB3	2.03	0.57
1:A:342:HIS:HD2	1:A:342:HIS:H	1.52	0.57
1:A:124:GLN:O	1:A:125:PRO:C	2.43	0.57
1:A:280:THR:HG23	1:A:584:ARG:NH1	2.19	0.57
1:A:44:THR:H	1:A:149:ASN:ND2	2.03	0.56
1:A:259:LEU:O	1:A:259:LEU:HD12	2.04	0.56
1:A:285:THR:O	1:A:287:ARG:N	2.37	0.56
1:A:280:THR:CG2	1:A:584:ARG:HD3	2.34	0.56
1:A:342:HIS:N	1:A:342:HIS:CD2	2.70	0.56
1:A:416:SER:OG	1:A:417:ALA:N	2.37	0.56
1:A:70:LEU:HD11	1:A:524:THR:HB	1.88	0.55
1:A:165:ILE:O	1:A:165:ILE:HD12	2.06	0.55
1:A:439:ASN:O	1:A:440:ASP:HB2	2.07	0.55
1:A:458:HIS:O	1:A:580:ARG:NH2	2.40	0.55
1:A:429:LEU:HD12	1:A:430:THR:N	2.21	0.55
1:A:79:GLU:HG3	1:A:516:LEU:CD2	2.36	0.55
1:A:219:ARG:HD3	1:A:219:ARG:C	2.27	0.54
1:A:284:GLN:HE22	1:A:587:TYR:N	1.97	0.54
1:A:155:VAL:HG22	1:A:520:VAL:HB	1.89	0.54
1:A:329:ILE:O	1:A:329:ILE:HG12	2.08	0.54
1:A:139:ASN:OD1	1:A:140:LEU:N	2.41	0.54
1:A:462:VAL:HG23	1:A:466:GLY:CA	2.37	0.53
1:A:202:PRO:HD2	1:A:203:TRP:CZ3	2.43	0.53
1:A:546:VAL:HG21	1:A:582:VAL:HG13	1.91	0.53
1:A:103:ALA:HB3	1:A:219:ARG:NH1	2.24	0.53
1:A:463:TYR:CB	1:A:464:PRO:CD	2.87	0.52
1:A:280:THR:OG1	1:A:584:ARG:HB3	2.09	0.52
1:A:225:TYR:O	1:A:227:ASN:N	2.42	0.52
1:A:320:MET:HB2	1:A:329:ILE:HD11	1.91	0.52
1:A:478:LYS:HB3	1:A:479:PRO:HD2	1.90	0.52
1:A:578:ILE:HD12	1:A:578:ILE:N	2.22	0.52
1:A:463:TYR:CD1	1:A:464:PRO:HD3	2.45	0.52
1:A:96:GLY:HA2	1:A:224:THR:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:PHE:CD2	1:A:200:PHE:N	2.78	0.51
1:A:414:ILE:HG13	1:A:443:PHE:HE1	1.75	0.51
1:A:113:LEU:HB3	1:A:498:LEU:HD23	1.91	0.51
1:A:259:LEU:HB2	1:A:263:ASP:HB2	1.93	0.50
1:A:280:THR:HG21	1:A:584:ARG:HD3	1.92	0.50
1:A:45:GLY:HA3	1:A:148:PHE:CE1	2.46	0.50
1:A:138:LEU:HD23	1:A:138:LEU:C	2.32	0.50
1:A:416:SER:O	1:A:418:PRO:O	2.30	0.50
1:A:552:GLU:O	1:A:561:VAL:HG13	2.11	0.50
1:A:141:VAL:HB	1:A:532:THR:O	2.12	0.50
1:A:183:ASN:HD22	1:A:183:ASN:N	2.10	0.49
1:A:206:THR:CG2	1:A:207:ILE:N	2.55	0.49
1:A:462:VAL:O	1:A:462:VAL:HG23	2.13	0.49
1:A:582:VAL:HG12	1:A:583:ALA:N	2.28	0.49
1:A:460:SER:HB3	1:A:580:ARG:NE	2.27	0.49
1:A:206:THR:HG23	1:A:381:GLN:HE22	1.77	0.49
1:A:92:THR:HB	1:A:235:ASN:HD21	1.78	0.49
1:A:112:SER:HA	1:A:210:PRO:HA	1.96	0.48
1:A:287:ARG:HA	1:A:332:ARG:HH21	1.79	0.48
1:A:464:PRO:HB2	1:A:465:GLN:CD	2.34	0.48
1:A:556:ASN:O	1:A:557:SER:C	2.52	0.48
1:A:165:ILE:C	1:A:165:ILE:HD12	2.34	0.48
1:A:239:THR:HB	1:A:240:PRO:HD2	1.96	0.48
1:A:69:ARG:NH1	1:A:199:GLY:O	2.47	0.48
1:A:225:TYR:O	1:A:226:GLU:C	2.51	0.48
1:A:285:THR:OG1	1:A:288:GLN:NE2	2.47	0.48
1:A:144:ASP:HB2	1:A:530:LYS:HB3	1.96	0.47
1:A:152:LEU:HD12	1:A:174:ALA:O	2.14	0.47
1:A:101:ASP:OD1	1:A:219:ARG:NH1	2.47	0.47
1:A:119:TRP:HA	1:A:468:ILE:HD11	1.97	0.47
1:A:287:ARG:C	1:A:332:ARG:HH21	2.17	0.47
1:A:322:VAL:HB	1:A:324:TRP:NE1	2.30	0.47
1:A:49:ASN:ND2	1:A:67:ALA:HA	2.30	0.47
1:A:384:GLU:HG3	1:A:394:GLU:HB2	1.95	0.47
1:A:56:LEU:HD13	1:A:56:LEU:N	2.30	0.47
1:A:480:ARG:O	1:A:481:LEU:HB3	2.14	0.46
1:A:79:GLU:HG3	1:A:516:LEU:HD23	1.96	0.46
1:A:256:ILE:CD1	1:A:256:ILE:N	2.71	0.46
1:A:326:SER:H	1:A:329:ILE:CG2	2.29	0.46
1:A:101:ASP:OD2	1:A:102:ASP:N	2.49	0.46
1:A:443:PHE:HD2	1:A:444:SER:H	1.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:LYS:N	1:A:438:LYS:HD2	2.30	0.46
1:A:327:GLU:OE1	1:A:327:GLU:HA	2.16	0.46
1:A:299:PRO:HG3	1:A:305:ALA:C	2.36	0.45
1:A:169:ASN:HD22	1:A:169:ASN:HA	1.59	0.45
1:A:362:ILE:CG2	1:A:368:LYS:HA	2.46	0.45
1:A:42:VAL:HG23	1:A:42:VAL:O	2.15	0.45
1:A:66:LEU:HA	1:A:66:LEU:HD23	1.77	0.45
1:A:207:ILE:C	1:A:207:ILE:HD12	2.37	0.45
1:A:423:PRO:HA	1:A:424:PRO:HD3	1.81	0.45
1:A:47:TYR:CE1	1:A:68:THR:HB	2.52	0.45
1:A:318:THR:HG22	1:A:330:ARG:HA	1.99	0.45
1:A:421:VAL:CG1	1:A:422:PRO:HD3	2.47	0.44
1:A:188:TYR:HA	1:A:496:GLN:NE2	2.32	0.44
1:A:79:GLU:HG3	1:A:516:LEU:HD21	1.99	0.44
1:A:206:THR:HG23	1:A:381:GLN:NE2	2.32	0.44
1:A:346:GLU:O	1:A:347:ALA:HB2	2.16	0.44
1:A:578:ILE:CD1	1:A:578:ILE:H	2.26	0.44
1:A:281:HIS:CD2	1:A:580:ARG:O	2.61	0.44
1:A:144:ASP:O	1:A:529:GLY:HA2	2.17	0.44
1:A:414:ILE:HG13	1:A:443:PHE:CE1	2.53	0.44
1:A:92:THR:CB	1:A:235:ASN:HD21	2.30	0.44
1:A:69:ARG:HE	1:A:202:PRO:HA	1.83	0.44
1:A:285:THR:C	1:A:287:ARG:N	2.71	0.43
1:A:433:ASN:HA	1:A:434:PRO:HD3	1.68	0.43
1:A:362:ILE:HG22	1:A:368:LYS:HA	2.00	0.43
1:A:326:SER:O	1:A:329:ILE:HG22	2.19	0.43
1:A:239:THR:HB	1:A:240:PRO:CD	2.48	0.43
1:A:176:MET:HB3	1:A:259:LEU:HD12	2.01	0.43
1:A:158:GLN:HG2	1:A:159:ASP:N	2.34	0.43
1:A:299:PRO:HB3	1:A:304:ASP:HB2	2.01	0.43
1:A:381:GLN:HG2	1:A:381:GLN:O	2.18	0.43
1:A:391:PRO:O	1:A:392:ALA:C	2.58	0.43
1:A:500:ARG:HH11	1:A:500:ARG:HG3	1.84	0.42
1:A:338:PHE:CD2	1:A:338:PHE:N	2.86	0.42
1:A:464:PRO:CD	1:A:576:PRO:HA	2.49	0.42
1:A:378:TYR:N	1:A:378:TYR:CD1	2.88	0.42
1:A:68:THR:HA	1:A:527:TRP:O	2.19	0.42
1:A:420:VAL:O	1:A:421:VAL:C	2.57	0.42
1:A:493:ALA:HB1	1:A:494:PRO:CD	2.48	0.42
1:A:70:LEU:HD12	1:A:71:VAL:N	2.35	0.42
1:A:293:PRO:HD3	1:A:327:GLU:OE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:TYR:CG	1:A:464:PRO:HD3	2.54	0.42
1:A:373:SER:HB3	1:A:398:TRP:O	2.19	0.42
1:A:86:VAL:O	1:A:103:ALA:HA	2.20	0.42
1:A:178:VAL:CG1	1:A:179:ALA:N	2.82	0.42
1:A:285:THR:H	1:A:288:GLN:HE22	1.66	0.42
1:A:265:PHE:CD1	1:A:265:PHE:C	2.93	0.42
1:A:155:VAL:HG12	1:A:168:TYR:CD2	2.54	0.42
1:A:421:VAL:CB	1:A:422:PRO:CD	2.79	0.41
1:A:49:ASN:ND2	1:A:68:THR:N	2.58	0.41
1:A:428:ILE:HG23	1:A:428:ILE:O	2.20	0.41
1:A:320:MET:CG	1:A:329:ILE:HD11	2.50	0.41
1:A:111:TRP:CE3	1:A:500:ARG:HB2	2.55	0.41
1:A:419:LEU:HG	1:A:420:VAL:N	2.36	0.41
1:A:119:TRP:CE2	1:A:468:ILE:HG12	2.56	0.41
1:A:49:ASN:HA	1:A:66:LEU:O	2.20	0.41
1:A:463:TYR:O	1:A:464:PRO:C	2.58	0.41
1:A:485:ALA:HA	1:A:486:PRO:HD3	1.88	0.41
1:A:431:ASN:ND2	1:A:442:HIS:HB2	2.36	0.40
1:A:463:TYR:CD1	1:A:464:PRO:CD	3.04	0.40
1:A:67:ALA:O	1:A:528:LYS:HA	2.21	0.40
1:A:207:ILE:CD1	1:A:207:ILE:C	2.89	0.40
1:A:376:TYR:O	1:A:395:ARG:HA	2.21	0.40
1:A:500:ARG:NH1	1:A:500:ARG:HG3	2.37	0.40
1:A:181:ASP:OD1	1:A:184:ASN:HA	2.21	0.40
1:A:301:ALA:O	1:A:303:THR:N	2.55	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	547/549 (100%)	490 (90%)	43 (8%)	14 (3%)	5 27

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	226	GLU
1	A	421	VAL
1	A	463	TYR
1	A	286	ASN
1	A	417	ALA
1	A	553	ASP
1	A	90	THR
1	A	302	ASP
1	A	349	ARG
1	A	125	PRO
1	A	233	GLU
1	A	557	SER
1	A	197	THR
1	A	486	PRO

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	471/471 (100%)	434 (92%)	37 (8%)	12	37

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LEU
1	A	98	MET
1	A	135	MET
1	A	138	LEU
1	A	140	LEU
1	A	149	ASN
1	A	169	ASN
1	A	193	ASN
1	A	195	MET
1	A	219	ARG
1	A	223	VAL

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Mol	Chain	Res	Type
1	A	229	GLU
1	A	249	THR
1	A	264	GLU
1	A	280	THR
1	A	286	ASN
1	A	288	GLN
1	A	295	LEU
1	A	325	VAL
1	A	327	GLU
1	A	331	THR
1	A	332	ARG
1	A	338	PHE
1	A	342	HIS
1	A	357	LYS
1	A	375	ARG
1	A	416	SER
1	A	418	PRO
1	A	433	ASN
1	A	438	LYS
1	A	443	PHE
1	A	465	GLN
1	A	500	ARG
1	A	512	ASN
1	A	552	GLU
1	A	554	ASN
1	A	569	THR

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	49	ASN
1	A	72	HIS
1	A	106	GLN
1	A	149	ASN
1	A	169	ASN
1	A	183	ASN
1	A	193	ASN
1	A	246	GLN
1	A	254	GLN
1	A	281	HIS
1	A	284	GLN
1	A	286	ASN

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Mol	Chain	Res	Type
1	A	288	GLN
1	A	291	GLN
1	A	342	HIS
1	A	381	GLN
1	A	431	ASN
1	A	433	ASN
1	A	465	GLN
1	A	467	GLN
1	A	496	GLN
1	A	554	ASN
1	A	573	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 carbohydrates 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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.