



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:02 AM UTC

PDB ID : 1Z14 / pdb_00001z14
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 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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

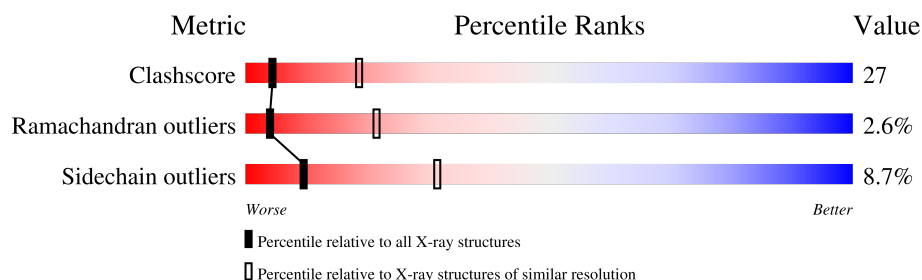
1 Overall quality at a glance

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	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (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 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 $\leq 5\%$.

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
			Total	C	N	O	S			
1	A	549	4317	2724	746	828	19	0	0	0

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.

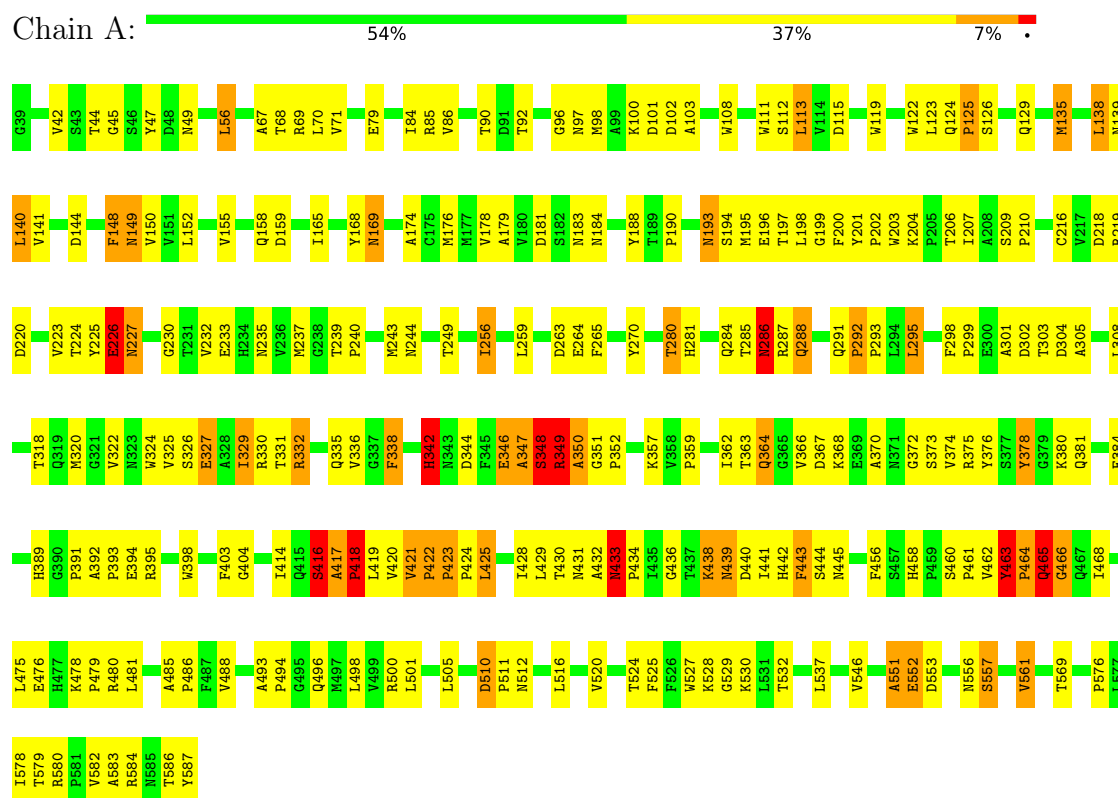
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	121	Total	O	0	0
			121	121		

3 Residue-property plots

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. 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	448.70Å 416.50Å 306.10Å 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	0.87	19/4441 (0.4%)	1.25	50/6073 (0.8%)

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 (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	347	ALA	CA-CB	-13.64	1.31	1.53
1	A	364	GLN	N-CA	12.73	1.62	1.46
1	A	350	ALA	CA-CB	-9.31	1.28	1.54
1	A	350	ALA	CA-C	-9.28	1.41	1.53
1	A	464	PRO	N-CD	-8.07	1.36	1.47
1	A	418	PRO	CA-C	-7.97	1.43	1.52
1	A	419	LEU	CA-C	-7.56	1.43	1.52
1	A	350	ALA	N-CA	-7.49	1.39	1.46
1	A	350	ALA	C-O	-7.39	1.16	1.24
1	A	348	SER	CA-C	-6.54	1.44	1.52
1	A	352	PRO	CA-C	-6.45	1.43	1.52
1	A	347	ALA	C-O	-5.96	1.16	1.23
1	A	352	PRO	C-O	-5.73	1.16	1.24
1	A	416	SER	CA-C	-5.61	1.45	1.53
1	A	226	GLU	C-N	-5.36	1.26	1.33
1	A	348	SER	C-O	-5.26	1.17	1.24
1	A	349	ARG	C-O	-5.12	1.17	1.24
1	A	346	GLU	C-O	-5.11	1.16	1.23
1	A	346	GLU	CA-C	-5.05	1.46	1.53

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	364	GLN	N-CA-C	-23.27	85.26	113.88
1	A	226	GLU	O-C-N	-13.72	104.35	122.59
1	A	226	GLU	CA-C-N	-11.66	103.69	121.53
1	A	226	GLU	C-N-CA	-11.66	103.69	121.53
1	A	226	GLU	CB-CG-CD	9.38	128.55	112.60
1	A	422	PRO	N-CA-C	-8.96	99.76	110.70
1	A	510	ASP	CA-C-N	8.58	129.10	119.32
1	A	510	ASP	C-N-CA	8.58	129.10	119.32
1	A	122	TRP	N-CA-C	8.11	121.66	111.69
1	A	439	ASN	N-CA-C	-7.99	99.32	110.35
1	A	201	TYR	CA-C-N	7.95	127.24	118.97
1	A	201	TYR	C-N-CA	7.95	127.24	118.97
1	A	456	PHE	N-CA-C	7.63	119.74	108.14
1	A	465	GLN	N-CA-C	7.46	122.41	113.16
1	A	216	CYS	N-CA-C	7.32	120.66	108.73
1	A	351	GLY	N-CA-C	-7.20	97.65	112.34
1	A	423	PRO	N-CA-C	7.18	119.46	110.70
1	A	372	GLY	N-CA-C	7.18	123.96	113.48
1	A	363	THR	CA-C-N	-7.11	110.14	122.36
1	A	363	THR	C-N-CA	-7.11	110.14	122.36
1	A	342	HIS	N-CA-C	6.83	120.96	109.76
1	A	505	LEU	N-CA-C	6.83	118.81	110.41
1	A	485	ALA	N-CA-C	6.76	116.10	108.25
1	A	374	VAL	N-CA-C	6.59	117.34	108.11
1	A	463	TYR	N-CA-C	6.59	124.38	109.81
1	A	204	LYS	CA-C-N	6.56	128.04	119.84
1	A	204	LYS	C-N-CA	6.56	128.04	119.84
1	A	378	TYR	N-CA-C	6.55	119.36	109.41
1	A	403	PHE	N-CA-C	6.53	118.40	111.28
1	A	364	GLN	N-CA-CB	6.53	119.27	110.59
1	A	148	PHE	N-CA-C	6.36	117.88	108.60
1	A	551	ALA	N-CA-C	-6.21	102.77	110.41
1	A	441	ILE	N-CA-CB	6.15	121.38	111.23
1	A	389	HIS	N-CA-C	6.10	119.49	109.85
1	A	432	ALA	N-CA-C	-6.04	105.15	113.18
1	A	227	ASN	CA-CB-CG	5.90	118.50	112.60
1	A	363	THR	CB-CA-C	-5.87	108.12	116.34
1	A	84	ILE	N-CA-C	5.81	116.24	108.11
1	A	123	LEU	N-CA-C	5.79	118.65	110.14
1	A	418	PRO	N-CA-C	-5.71	102.48	111.34
1	A	227	ASN	N-CA-C	-5.41	104.03	110.41
1	A	436	GLY	N-CA-C	-5.41	100.36	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	GLY	N-CA-C	-5.41	106.10	111.56
1	A	433	ASN	CA-C-N	5.41	126.60	119.84
1	A	433	ASN	C-N-CA	5.41	126.60	119.84
1	A	292	PRO	CA-C-N	5.32	126.49	119.84
1	A	292	PRO	C-N-CA	5.32	126.49	119.84
1	A	347	ALA	N-CA-C	5.25	116.49	108.52
1	A	466	GLY	N-CA-C	5.14	118.78	112.14
1	A	113	LEU	N-CA-C	5.13	117.19	109.23

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	224	0
2	A	121	0	0	0	0
All	All	4438	0	4123	224	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 27.

All (224) 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	1.17
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	0.97
1:A:295:LEU:HD12	1:A:295:LEU:H	1.30	0.94
1:A:284:GLN:HE21	1:A:586:THR:H	0.94	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:TYR:HB3	1:A:464:PRO:HD3	1.52	0.92
1:A:284:GLN:HE22	1:A:587:TYR:H	1.17	0.91
1:A:433:ASN:N	1:A:433:ASN:HD22	1.66	0.91
1:A:49:ASN:HD22	1:A:68:THR:H	1.17	0.90
1:A:421:VAL:CB	1:A:422:PRO:HD3	2.02	0.89
1:A:206:THR:HG22	1:A:207:ILE:N	1.85	0.86
1:A:417:ALA:HB3	1:A:418:PRO:CD	2.09	0.83
1:A:286:ASN:HD21	1:A:335:GLN:HA	1.44	0.82
1:A:421:VAL:HB	1:A:422:PRO:CD	2.10	0.81
1:A:49:ASN:ND2	1:A:68:THR:H	1.79	0.81
1:A:206:THR:CG2	1:A:207:ILE:H	1.96	0.77
1:A:286:ASN:HD22	1:A:336:VAL:H	1.30	0.77
1:A:367:ASP:HB3	1:A:370:ALA:HB3	1.66	0.76
1:A:280:THR:HG23	1:A:584:ARG:HH11	1.50	0.76
1:A:551:ALA:HB1	1:A:561:VAL:HG12	1.69	0.75
1:A:342:HIS:H	1:A:342:HIS:CD2	2.02	0.75
1:A:284:GLN:HE21	1:A:586:THR:N	1.78	0.74
1:A:256:ILE:N	1:A:256:ILE:HD12	2.02	0.74
1:A:69:ARG:HH21	1:A:202:PRO:HG3	1.52	0.74
1:A:281:HIS:HD2	1:A:580:ARG:O	1.71	0.74
1:A:285:THR:H	1:A:288:GLN:NE2	1.84	0.74
1:A:69:ARG:NH2	1:A:202:PRO:HG3	2.04	0.73
1:A:295:LEU:HD12	1:A:295:LEU:N	2.03	0.73
1:A:463:TYR:CB	1:A:464:PRO:HD3	2.17	0.72
1:A:219:ARG:HD3	1:A:220:ASP:N	2.04	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:115:ASP:O	1:A:198:LEU:HD13	1.91	0.71
1:A:342:HIS:HD2	1:A:445:ASN:HA	1.56	0.71
1:A:500:ARG:HD3	1:A:501:LEU:O	1.93	0.68
1:A:578:ILE:HD12	1:A:578:ILE:H	1.56	0.68
1:A:286:ASN:ND2	1:A:336:VAL:H	1.91	0.67
1:A:380:LYS:HA	1:A:384:GLU:HB3	1.75	0.67
1:A:295:LEU:H	1:A:295:LEU:CD1	2.05	0.66
1:A:113:LEU:HD23	1:A:209:SER:O	1.95	0.66
1:A:348:SER:O	1:A:350:ALA:N	2.28	0.66
1:A:284:GLN:NE2	1:A:586:THR:N	2.40	0.65
1:A:342:HIS:CD2	1:A:445:ASN:HA	2.31	0.64
1:A:150:VAL:HG21	1:A:259:LEU:HD13	1.78	0.64
1:A:207:ILE:HD12	1:A:207:ILE:O	1.97	0.64
1:A:462:VAL:HG23	1:A:466:GLY:HA3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:ALA:CB	1:A:418:PRO:HD3	2.28	0.63
1:A:45:GLY:HA3	1:A:148:PHE:CD1	2.33	0.63
1:A:135:MET:SD	1:A:537:LEU:HD23	2.39	0.63
1:A:443:PHE:CD2	1:A:444:SER:N	2.67	0.62
1:A:433:ASN:N	1:A:433:ASN:ND2	2.37	0.62
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	0.61
1:A:425:LEU:C	1:A:425:LEU:HD13	2.24	0.61
1:A:176:MET:HE1	1:A:525:PHE:CE2	2.34	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	0.60
1:A:219:ARG:HD3	1:A:219:ARG:C	2.27	0.60
1:A:124:GLN:O	1:A:125:PRO:C	2.43	0.60
1:A:284:GLN:NE2	1:A:587:TYR:H	1.93	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
1:A:433:ASN:HD22	1:A:433:ASN:H	1.44	0.59
1:A:194:SER:HB2	1:A:196:GLU:HG3	1.84	0.59
1:A:256:ILE:HD12	1:A:256:ILE:H	1.68	0.59
1:A:126:SER:O	1:A:129:GLN:HB3	2.03	0.58
1:A:218:ASP:OD1	1:A:349:ARG:NH1	2.35	0.58
1:A:280:THR:CG2	1:A:584:ARG:HD3	2.34	0.58
1:A:178:VAL:HG12	1:A:179:ALA:N	2.18	0.57
1:A:85:ARG:HD2	1:A:237:MET:HG2	1.85	0.57
1:A:417:ALA:HB3	1:A:418:PRO:HD2	1.83	0.57
1:A:259:LEU:HD12	1:A:259:LEU:O	2.04	0.57
1:A:342:HIS:CD2	1:A:342:HIS:N	2.70	0.57
1:A:342:HIS:H	1:A:342:HIS:HD2	1.52	0.57
1:A:285:THR:O	1:A:287:ARG:N	2.37	0.57
1:A:416:SER:OG	1:A:417:ALA:N	2.37	0.56
1:A:44:THR:H	1:A:149:ASN:ND2	2.03	0.56
1:A:417:ALA:HB3	1:A:418:PRO:HD3	1.84	0.56
1:A:165:ILE:HD12	1:A:165:ILE:O	2.06	0.56
1:A:429:LEU:HD12	1:A:430:THR:N	2.21	0.56
1:A:79:GLU:HG3	1:A:516:LEU:CD2	2.37	0.55
1:A:138:LEU:C	1:A:138:LEU:HD23	2.32	0.55
1:A:439:ASN:O	1:A:440:ASP:HB2	2.07	0.55
1:A:578:ILE:HD12	1:A:578:ILE:N	2.22	0.55
1:A:70:LEU:HD11	1:A:524:THR:HB	1.88	0.55
1:A:280:THR:HG23	1:A:584:ARG:NH1	2.19	0.55
1:A:155:VAL:HG22	1:A:520:VAL:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:HIS:O	1:A:580:ARG:NH2	2.40	0.54
1:A:462:VAL:HG23	1:A:466:GLY:CA	2.37	0.54
1:A:464:PRO:HB2	1:A:465:GLN:CD	2.34	0.53
1:A:103:ALA:HB3	1:A:219:ARG:NH1	2.24	0.53
1:A:284:GLN:HE22	1:A:587:TYR:N	1.97	0.53
1:A:329:ILE:HG12	1:A:329:ILE:O	2.08	0.53
1:A:139:ASN:OD1	1:A:140:LEU:N	2.41	0.53
1:A:202:PRO:HD2	1:A:203:TRP:CZ3	2.43	0.53
1:A:225:TYR:O	1:A:226:GLU:C	2.51	0.53
1:A:478:LYS:HB3	1:A:479:PRO:HD2	1.90	0.53
1:A:225:TYR:O	1:A:227:ASN:N	2.42	0.53
1:A:165:ILE:HD12	1:A:165:ILE:C	2.34	0.52
1:A:280:THR:OG1	1:A:584:ARG:HB3	2.09	0.52
1:A:556:ASN:O	1:A:557:SER:C	2.52	0.52
1:A:463:TYR:CD1	1:A:464:PRO:HD3	2.45	0.52
1:A:287:ARG:C	1:A:332:ARG:HH21	2.17	0.52
1:A:546:VAL:HG21	1:A:582:VAL:HG13	1.91	0.52
1:A:96:GLY:HA2	1:A:224:THR:O	2.10	0.51
1:A:200:PHE:N	1:A:200:PHE:CD2	2.78	0.51
1:A:113:LEU:HB3	1:A:498:LEU:HD23	1.91	0.51
1:A:280:THR:HG21	1:A:584:ARG:HD3	1.92	0.51
1:A:320:MET:HB2	1:A:329:ILE:HD11	1.91	0.51
1:A:45:GLY:HA3	1:A:148:PHE:CE1	2.46	0.51
1:A:299:PRO:HG3	1:A:305:ALA:C	2.36	0.51
1:A:259:LEU:HB2	1:A:263:ASP:HB2	1.93	0.50
1:A:552:GLU:O	1:A:561:VAL:HG13	2.11	0.50
1:A:416:SER:O	1:A:418:PRO:O	2.30	0.50
1:A:414:ILE:HG13	1:A:443:PHE:HE1	1.75	0.50
1:A:207:ILE:HD12	1:A:207:ILE:C	2.37	0.49
1:A:206:THR:HG23	1:A:381:GLN:HE22	1.77	0.49
1:A:462:VAL:HG23	1:A:462:VAL:O	2.13	0.49
1:A:582:VAL:HG12	1:A:583:ALA:N	2.28	0.49
1:A:443:PHE:HD2	1:A:444:SER:H	1.61	0.48
1:A:183:ASN:N	1:A:183:ASN:HD22	2.10	0.48
1:A:285:THR:C	1:A:287:ARG:N	2.71	0.48
1:A:460:SER:HB3	1:A:580:ARG:NE	2.27	0.48
1:A:141:VAL:HB	1:A:532:THR:O	2.12	0.48
1:A:144:ASP:HB2	1:A:530:LYS:HB3	1.96	0.48
1:A:239:THR:HB	1:A:240:PRO:HD2	1.96	0.48
1:A:256:ILE:N	1:A:256:ILE:CD1	2.71	0.48
1:A:287:ARG:HA	1:A:332:ARG:HH21	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:ILE:H	1:A:578:ILE:CD1	2.26	0.48
1:A:112:SER:HA	1:A:210:PRO:HA	1.96	0.47
1:A:69:ARG:NH1	1:A:199:GLY:O	2.47	0.47
1:A:285:THR:OG1	1:A:288:GLN:NE2	2.47	0.47
1:A:384:GLU:HG3	1:A:394:GLU:HB2	1.95	0.47
1:A:420:VAL:O	1:A:421:VAL:C	2.57	0.47
1:A:101:ASP:OD1	1:A:219:ARG:NH1	2.47	0.47
1:A:463:TYR:CB	1:A:464:PRO:CD	2.87	0.47
1:A:152:LEU:HD12	1:A:174:ALA:O	2.14	0.47
1:A:322:VAL:HB	1:A:324:TRP:NE1	2.30	0.47
1:A:391:PRO:O	1:A:392:ALA:C	2.58	0.47
1:A:438:LYS:HD2	1:A:438:LYS:N	2.30	0.47
1:A:480:ARG:O	1:A:481:LEU:HB3	2.14	0.47
1:A:92:THR:HB	1:A:235:ASN:HD21	1.78	0.47
1:A:176:MET:HE1	1:A:525:PHE:CD2	2.50	0.47
1:A:79:GLU:HG3	1:A:516:LEU:HD23	1.96	0.47
1:A:42:VAL:HG23	1:A:42:VAL:O	2.15	0.46
1:A:265:PHE:CD1	1:A:265:PHE:C	2.93	0.46
1:A:98:MET:HE2	1:A:98:MET:HB2	1.79	0.46
1:A:56:LEU:HD13	1:A:56:LEU:N	2.30	0.46
1:A:119:TRP:HA	1:A:468:ILE:HD11	1.97	0.46
1:A:346:GLU:O	1:A:347:ALA:HB2	2.16	0.46
1:A:49:ASN:ND2	1:A:67:ALA:HA	2.30	0.46
1:A:326:SER:H	1:A:329:ILE:CG2	2.29	0.45
1:A:463:TYR:O	1:A:464:PRO:C	2.58	0.45
1:A:47:TYR:CE1	1:A:68:THR:HB	2.52	0.45
1:A:327:GLU:HA	1:A:327:GLU:OE1	2.16	0.45
1:A:362:ILE:CG2	1:A:368:LYS:HA	2.46	0.45
1:A:101:ASP:OD2	1:A:102:ASP:N	2.49	0.45
1:A:207:ILE:C	1:A:207:ILE:CD1	2.89	0.45
1:A:318:THR:HG22	1:A:330:ARG:HA	1.98	0.45
1:A:92:THR:CB	1:A:235:ASN:HD21	2.30	0.45
1:A:188:TYR:HA	1:A:496:GLN:NE2	2.32	0.45
1:A:463:TYR:HB3	1:A:464:PRO:CD	2.35	0.45
1:A:206:THR:HG23	1:A:381:GLN:NE2	2.32	0.45
1:A:144:ASP:O	1:A:529:GLY:HA2	2.17	0.45
1:A:421:VAL:CG1	1:A:422:PRO:HD3	2.47	0.44
1:A:243:MET:C	1:A:244:ASN:OD1	2.60	0.44
1:A:79:GLU:HG3	1:A:516:LEU:HD21	1.99	0.44
1:A:49:ASN:ND2	1:A:68:THR:N	2.58	0.44
1:A:226:GLU:O	1:A:227:ASN:CG	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:GLN:C	1:A:366:VAL:H	2.26	0.44
1:A:423:PRO:HA	1:A:424:PRO:HD3	1.81	0.44
1:A:69:ARG:HE	1:A:202:PRO:HA	1.83	0.44
1:A:108:TRP:CD1	1:A:108:TRP:C	2.96	0.44
1:A:338:PHE:N	1:A:338:PHE:CD2	2.86	0.44
1:A:493:ALA:HB1	1:A:494:PRO:CD	2.48	0.43
1:A:239:THR:HB	1:A:240:PRO:CD	2.48	0.43
1:A:362:ILE:HG22	1:A:368:LYS:HA	2.00	0.43
1:A:169:ASN:HD22	1:A:169:ASN:HA	1.59	0.43
1:A:326:SER:O	1:A:329:ILE:HG22	2.19	0.43
1:A:381:GLN:O	1:A:381:GLN:HG2	2.18	0.43
1:A:373:SER:HB3	1:A:398:TRP:O	2.19	0.43
1:A:344:ASP:OD2	1:A:344:ASP:C	2.61	0.43
1:A:414:ILE:HG13	1:A:443:PHE:CE1	2.52	0.43
1:A:500:ARG:HG3	1:A:500:ARG:HH11	1.84	0.43
1:A:68:THR:HA	1:A:527:TRP:O	2.19	0.42
1:A:158:GLN:HG2	1:A:159:ASP:N	2.34	0.42
1:A:155:VAL:HG12	1:A:168:TYR:CD2	2.54	0.42
1:A:178:VAL:CG1	1:A:179:ALA:N	2.82	0.42
1:A:281:HIS:CD2	1:A:580:ARG:O	2.61	0.42
1:A:421:VAL:CB	1:A:422:PRO:CD	2.79	0.42
1:A:97:ASN:O	1:A:98:MET:C	2.62	0.42
1:A:501:LEU:HD23	1:A:501:LEU:HA	1.84	0.42
1:A:176:MET:HB3	1:A:259:LEU:HD12	2.00	0.42
1:A:299:PRO:HB3	1:A:304:ASP:HB2	2.01	0.42
1:A:464:PRO:CD	1:A:576:PRO:HA	2.49	0.42
1:A:285:THR:O	1:A:286:ASN:C	2.62	0.42
1:A:291:GLN:HA	1:A:292:PRO:HD2	1.92	0.42
1:A:378:TYR:CD1	1:A:378:TYR:N	2.88	0.42
1:A:70:LEU:HD12	1:A:71:VAL:N	2.35	0.42
1:A:320:MET:CG	1:A:329:ILE:HD11	2.50	0.42
1:A:463:TYR:CG	1:A:464:PRO:HD3	2.54	0.42
1:A:285:THR:C	1:A:287:ARG:H	2.29	0.41
1:A:111:TRP:CE3	1:A:500:ARG:HB2	2.55	0.41
1:A:525:PHE:CD1	1:A:525:PHE:C	2.99	0.41
1:A:293:PRO:HD3	1:A:327:GLU:OE2	2.20	0.41
1:A:301:ALA:C	1:A:303:THR:H	2.29	0.41
1:A:270:TYR:CD1	1:A:270:TYR:C	2.98	0.41
1:A:428:ILE:HG23	1:A:428:ILE:O	2.20	0.41
1:A:392:ALA:HA	1:A:393:PRO:HD3	1.90	0.41
1:A:465:GLN:CD	1:A:465:GLN:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:PRO:HA	1:A:293:PRO:HD3	1.84	0.41
1:A:376:TYR:O	1:A:395:ARG:HA	2.21	0.41
1:A:67:ALA:O	1:A:528:LYS:HA	2.21	0.41
1:A:475:LEU:O	1:A:476:GLU:C	2.63	0.41
1:A:510:ASP:HA	1:A:511:PRO:HD3	1.79	0.41
1:A:86:VAL:O	1:A:103:ALA:HA	2.20	0.41
1:A:181:ASP:OD1	1:A:184:ASN:HA	2.21	0.41
1:A:298:PHE:HA	1:A:299:PRO:HD3	1.97	0.41
1:A:119:TRP:CE2	1:A:468:ILE:HG12	2.56	0.40
1:A:285:THR:H	1:A:288:GLN:HE22	1.66	0.40
1:A:433:ASN:HA	1:A:434:PRO:HD3	1.68	0.40
1:A:463:TYR:CD1	1:A:464:PRO:CD	3.04	0.40
1:A:500:ARG:HG3	1:A:500:ARG:NH1	2.37	0.40
1:A:431:ASN:ND2	1:A:442:HIS:HB2	2.36	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%)	4 21

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

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Mol	Chain	Res	Type
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%)	430 (91%)	41 (9%)	9 31

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LEU
1	A	100	LYS
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	223	VAL
1	A	232	VAL
1	A	249	THR
1	A	256	ILE
1	A	264	GLU
1	A	280	THR
1	A	286	ASN
1	A	288	GLN
1	A	295	LEU
1	A	308	LEU

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Mol	Chain	Res	Type
1	A	325	VAL
1	A	327	GLU
1	A	329	ILE
1	A	331	THR
1	A	332	ARG
1	A	338	PHE
1	A	342	HIS
1	A	357	LYS
1	A	359	PRO
1	A	375	ARG
1	A	416	SER
1	A	418	PRO
1	A	425	LEU
1	A	433	ASN
1	A	438	LYS
1	A	443	PHE
1	A	465	GLN
1	A	488	VAL
1	A	512	ASN
1	A	552	GLU
1	A	561	VAL
1	A	569	THR

Sometimes 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	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
1	A	288	GLN
1	A	291	GLN
1	A	335	GLN
1	A	342	HIS
1	A	381	GLN
1	A	431	ASN

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Mol	Chain	Res	Type
1	A	433	ASN
1	A	465	GLN
1	A	467	GLN
1	A	496	GLN
1	A	554	ASN
1	A	571	ASN
1	A	573	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 oligosaccharides 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

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.