Full wwPDB X-ray Structure Validation Report (i)

Oct 17, 2021 – 12:17 AM EDT

PDB ID	:	1P5Y
Title	:	The structures of host range controlling regions of the capsids of canine and feline parvoviruses and mutants
Authors	:	Agbandje-McKenna, M.; Govindasamy, L.
Deposited on	:	2003-04-28
Resolution	:	3.20 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 following versions of software and data (see references (i)) were used in the production of this report:

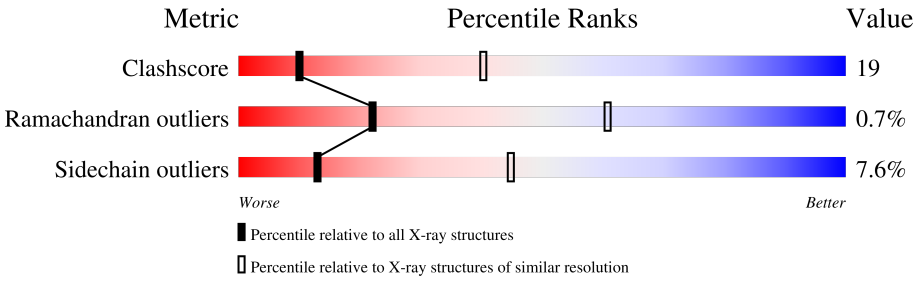
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 3.20 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	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	548	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4393 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 Coat protein VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	545	4328	2751	738	823	16	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	GLU	TYR	SEE REMARK 999	UNP P30129
A	93	ASP	ASN	engineered mutation	UNP P30129

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	65	65	65	0	0

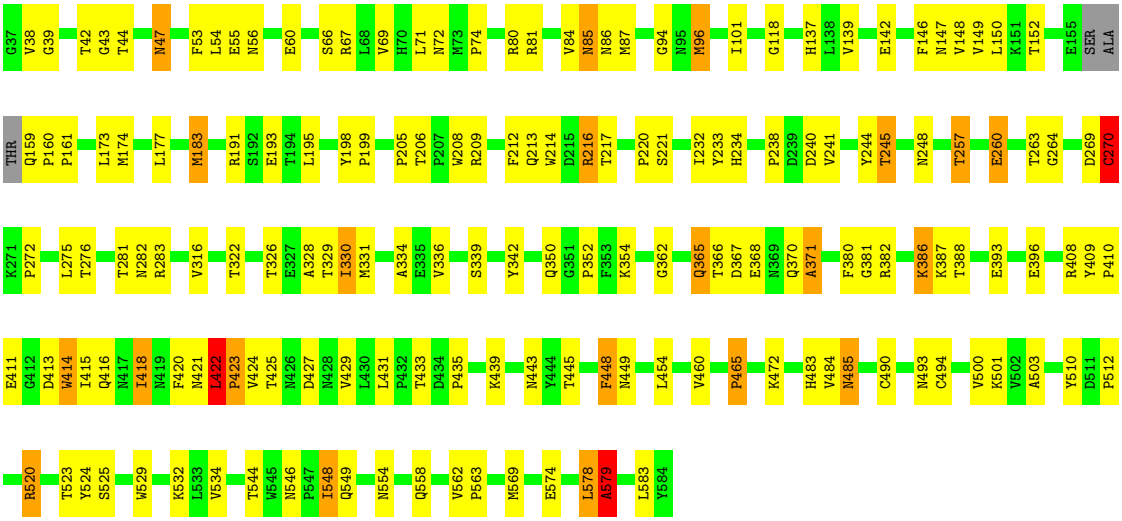
3 Residue-property plots (i)

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. 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: Coat protein VP2

Chain A:



4 Data and refinement statistics (i)

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	440.45Å 246.81Å 443.65Å 90.00° 93.54° 90.00°	Depositor
Resolution (Å)	25.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (25.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.252 , 0.253	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4393	wwPDB-VP
Average B, all atoms (Å^2)	37.0	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	0.95	2/4456 (0.0%)	0.79	10/6092 (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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	423	PRO	N-CD	-47.28	0.81	1.47
1	A	423	PRO	N-CA	28.88	1.96	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	423	PRO	N-CD-CG	16.95	128.62	103.20
1	A	423	PRO	N-CA-CB	-8.84	92.70	103.30
1	A	422	LEU	C-N-CD	7.15	143.42	128.40
1	A	270	CYS	C-N-CA	6.79	138.67	121.70
1	A	448	PHE	CB-CG-CD2	-6.69	116.12	120.80
1	A	579	ALA	C-N-CD	-6.62	106.03	120.60
1	A	423	PRO	CA-N-CD	-6.31	102.66	111.50
1	A	423	PRO	N-CA-C	6.31	128.50	112.10
1	A	421	ASN	O-C-N	6.30	132.78	122.70
1	A	422	LEU	CA-C-N	5.10	131.38	117.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	422	LEU	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	A	4328	0	4128	161	0
2	A	65	0	0	5	0
All	All	4393	0	4128	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 19.

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:423:PRO:N	1:A:423:PRO:CA	1.96	1.29
1:A:422:LEU:C	1:A:423:PRO:CD	2.04	1.24
1:A:423:PRO:N	1:A:423:PRO:CG	2.10	1.13
1:A:193:GLU:HB3	1:A:206:THR:HG21	1.30	1.09
1:A:423:PRO:N	1:A:423:PRO:HD3	1.42	1.06
1:A:423:PRO:N	1:A:423:PRO:HD2	1.42	1.04
1:A:245:THR:HG22	1:A:248:ASN:H	1.29	0.96
1:A:423:PRO:N	1:A:423:PRO:CD	0.81	0.96
1:A:485:ASN:H	1:A:485:ASN:HD22	0.96	0.94
1:A:101:ILE:HD13	1:A:216:ARG:HH12	1.32	0.93
1:A:85:ASN:HD21	1:A:87:MET:HG3	1.37	0.90
1:A:485:ASN:HD22	1:A:485:ASN:N	1.71	0.89
1:A:282:ASN:HD21	1:A:336:VAL:H	1.18	0.87
1:A:485:ASN:H	1:A:485:ASN:ND2	1.74	0.84
1:A:418:ILE:HD12	1:A:418:ILE:H	1.41	0.84
1:A:85:ASN:HD22	1:A:86:ASN:N	1.76	0.81
1:A:42:THR:CG2	1:A:147:ASN:H	1.95	0.79
1:A:42:THR:HG23	1:A:147:ASN:H	1.45	0.79
1:A:326:THR:HG23	1:A:328:ALA:H	1.50	0.77
1:A:85:ASN:HD22	1:A:85:ASN:C	1.87	0.76
1:A:269:ASP:OD1	1:A:270:CYS:N	2.17	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ASN:ND2	1:A:66:SER:H	1.84	0.75
1:A:483:HIS:HB3	1:A:485:ASN:ND2	2.02	0.75
1:A:483:HIS:HB3	1:A:485:ASN:HD21	1.51	0.75
1:A:282:ASN:ND2	1:A:336:VAL:H	1.86	0.73
1:A:423:PRO:N	1:A:423:PRO:CB	2.54	0.71
1:A:422:LEU:C	1:A:423:PRO:CA	2.58	0.70
1:A:71:LEU:HD22	1:A:500:VAL:CG1	2.21	0.69
1:A:174:MET:HE2	1:A:503:ALA:HA	1.77	0.67
1:A:424:VAL:CG2	1:A:429:VAL:HG13	2.25	0.67
1:A:326:THR:HG22	1:A:329:THR:OG1	1.94	0.67
1:A:85:ASN:ND2	1:A:87:MET:H	1.95	0.65
1:A:276:THR:HA	2:A:598:HOH:O	1.95	0.65
1:A:54:LEU:HD11	1:A:60:GLU:HB2	1.78	0.64
1:A:424:VAL:HG21	1:A:429:VAL:HG13	1.80	0.63
1:A:578:LEU:O	1:A:579:ALA:HB3	1.99	0.62
1:A:418:ILE:HD12	1:A:418:ILE:N	2.12	0.61
1:A:443:ASN:ND2	1:A:445:THR:H	1.99	0.61
1:A:418:ILE:H	1:A:418:ILE:CD1	2.05	0.60
1:A:424:VAL:HG21	1:A:429:VAL:CG1	2.32	0.59
1:A:81:ARG:HH11	1:A:81:ARG:HB3	1.67	0.59
1:A:583:LEU:O	1:A:583:LEU:HD23	2.02	0.59
1:A:42:THR:OG1	1:A:260:GLU:HB3	2.02	0.59
1:A:282:ASN:HD21	1:A:336:VAL:N	1.93	0.58
1:A:149:VAL:C	1:A:150:LEU:HD12	2.24	0.58
1:A:316:VAL:O	1:A:330:ILE:HD13	2.04	0.58
1:A:414:TRP:HE1	1:A:416:GLN:HE21	1.52	0.58
1:A:578:LEU:O	1:A:579:ALA:CB	2.52	0.58
1:A:213:GLN:HG3	1:A:240:ASP:CB	2.34	0.57
1:A:42:THR:H	1:A:147:ASN:ND2	2.03	0.57
1:A:562:VAL:HG13	1:A:563:PRO:HD2	1.85	0.57
1:A:101:ILE:HD13	1:A:216:ARG:NH1	2.14	0.57
1:A:96:MET:N	1:A:96:MET:HE2	2.20	0.56
1:A:238:PRO:HA	1:A:241:VAL:HG23	1.88	0.56
1:A:326:THR:HG23	1:A:328:ALA:N	2.18	0.56
1:A:96:MET:HE2	1:A:96:MET:H	1.71	0.56
1:A:388:THR:HB	1:A:569:MET:H	1.71	0.55
1:A:183:MET:HE2	1:A:183:MET:HA	1.87	0.55
1:A:183:MET:HG3	1:A:208:TRP:HH2	1.69	0.55
1:A:71:LEU:HD22	1:A:500:VAL:HG12	1.89	0.55
1:A:85:ASN:ND2	1:A:87:MET:HG3	2.16	0.55
1:A:38:VAL:HG13	1:A:39:GLY:N	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:MET:CG	1:A:208:TRP:CH2	2.90	0.54
1:A:422:LEU:O	1:A:423:PRO:CA	2.56	0.54
1:A:213:GLN:HG3	1:A:240:ASP:HB2	1.89	0.54
1:A:336:VAL:O	1:A:408:ARG:NH2	2.41	0.54
1:A:435:PRO:HB3	1:A:439:LYS:O	2.08	0.53
1:A:183:MET:HG2	1:A:208:TRP:CH2	2.43	0.53
1:A:43:GLY:HA3	1:A:146:PHE:CD2	2.43	0.53
1:A:263:THR:HG22	1:A:264:GLY:N	2.24	0.53
1:A:443:ASN:HD22	1:A:445:THR:H	1.55	0.53
1:A:174:MET:CE	1:A:503:ALA:HA	2.39	0.52
1:A:42:THR:HG23	1:A:146:PHE:HB2	1.91	0.52
1:A:53:PHE:C	1:A:54:LEU:HD12	2.30	0.52
1:A:579:ALA:C	2:A:598:HOH:O	2.47	0.52
1:A:472:LYS:HA	1:A:494:CYS:SG	2.50	0.52
1:A:183:MET:HA	1:A:183:MET:CE	2.40	0.52
1:A:365:GLN:HG2	1:A:409:TYR:CE2	2.45	0.51
1:A:424:VAL:HG22	1:A:429:VAL:HG13	1.93	0.51
1:A:137:HIS:CE1	1:A:272:PRO:HB3	2.46	0.51
1:A:142:GLU:HG2	1:A:532:LYS:HB3	1.92	0.51
1:A:232:ILE:HG22	1:A:233:TYR:N	2.26	0.50
1:A:460:VAL:HG21	1:A:484:VAL:HA	1.92	0.50
1:A:96:MET:HG2	1:A:220:PRO:HA	1.94	0.50
1:A:382:ARG:HG3	1:A:386:LYS:HG2	1.94	0.50
1:A:137:HIS:NE2	1:A:272:PRO:HB3	2.26	0.50
1:A:367:ASP:C	1:A:368:GLU:HG2	2.31	0.50
1:A:578:LEU:N	1:A:578:LEU:HD23	2.27	0.50
1:A:485:ASN:N	1:A:485:ASN:ND2	2.45	0.49
1:A:183:MET:HG3	1:A:208:TRP:CH2	2.47	0.49
1:A:431:LEU:C	1:A:433:THR:H	2.15	0.48
1:A:217:THR:OG1	1:A:234:HIS:HE1	1.97	0.48
1:A:362:GLY:HA2	1:A:366:THR:HG21	1.95	0.48
1:A:38:VAL:HG13	1:A:39:GLY:H	1.77	0.48
1:A:54:LEU:HD12	1:A:54:LEU:N	2.28	0.47
1:A:322:THR:HG21	1:A:420:PHE:HD2	1.79	0.47
1:A:173:LEU:HD11	1:A:500:VAL:HG13	1.95	0.47
1:A:216:ARG:C	1:A:216:ARG:HD3	2.35	0.47
1:A:150:LEU:HD12	1:A:150:LEU:N	2.29	0.47
1:A:352:PRO:HG3	2:A:594:HOH:O	2.14	0.47
1:A:386:LYS:HG3	1:A:387:LYS:N	2.29	0.47
1:A:410:PRO:HA	1:A:413:ASP:OD2	2.14	0.47
1:A:85:ASN:HA	1:A:101:ILE:HG13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:SER:O	1:A:449:ASN:HA	2.15	0.47
1:A:554:ASN:O	1:A:558:GLN:HB2	2.15	0.47
1:A:510:TYR:CE2	1:A:512:PRO:HG3	2.50	0.46
1:A:74:PRO:O	1:A:520:ARG:NH2	2.46	0.46
1:A:380:PHE:N	1:A:380:PHE:CD1	2.83	0.46
1:A:245:THR:CG2	1:A:248:ASN:H	2.14	0.46
1:A:174:MET:HE1	1:A:501:LYS:CE	2.45	0.46
1:A:367:ASP:O	1:A:368:GLU:HG2	2.15	0.46
1:A:160:PRO:HB2	1:A:161:PRO:CA	2.46	0.46
1:A:84:VAL:O	1:A:101:ILE:HA	2.16	0.45
1:A:583:LEU:HD23	1:A:583:LEU:C	2.35	0.45
1:A:544:THR:HB	1:A:546:ASN:ND2	2.31	0.45
1:A:579:ALA:O	2:A:598:HOH:O	2.21	0.45
1:A:148:VAL:O	1:A:257:THR:HG23	2.17	0.45
1:A:159:GLN:N	1:A:160:PRO:CD	2.79	0.45
1:A:85:ASN:HD21	1:A:87:MET:H	1.64	0.45
1:A:548:ILE:HG13	1:A:579:ALA:HA	1.99	0.45
1:A:269:ASP:CG	1:A:270:CYS:N	2.70	0.45
1:A:85:ASN:C	1:A:85:ASN:ND2	2.60	0.44
1:A:425:THR:HG22	1:A:427:ASP:H	1.83	0.44
1:A:193:GLU:CB	1:A:206:THR:HG21	2.22	0.44
1:A:367:ASP:O	1:A:368:GLU:CG	2.66	0.44
1:A:281:THR:HG23	1:A:283:ARG:H	1.82	0.44
1:A:330:ILE:HD13	1:A:331:MET:H	1.82	0.44
1:A:484:VAL:O	1:A:484:VAL:HG12	2.18	0.44
1:A:69:VAL:CG1	1:A:205:PRO:HD3	2.47	0.44
1:A:334:ALA:HB1	1:A:454:LEU:O	2.17	0.44
1:A:118:GLY:CA	1:A:465:PRO:HB2	2.48	0.43
1:A:411:GLU:OE1	1:A:411:GLU:N	2.39	0.43
1:A:94:GLY:HA2	1:A:221:SER:O	2.18	0.43
1:A:409:TYR:CE1	1:A:411:GLU:HB2	2.54	0.43
1:A:81:ARG:HB3	1:A:81:ARG:NH1	2.31	0.43
1:A:414:TRP:HE1	1:A:416:GLN:HG3	1.82	0.43
1:A:198:TYR:HA	1:A:199:PRO:HD3	1.93	0.42
1:A:326:THR:CG2	1:A:329:THR:H	2.32	0.42
1:A:183:MET:CE	1:A:244:TYR:HB3	2.49	0.42
1:A:409:TYR:CZ	1:A:411:GLU:HB2	2.55	0.42
1:A:579:ALA:HB3	2:A:598:HOH:O	2.17	0.42
1:A:139:VAL:HB	1:A:534:VAL:O	2.20	0.42
1:A:548:ILE:HG23	1:A:549:GLN:N	2.34	0.42
1:A:66:SER:HA	1:A:529:TRP:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ARG:HH11	1:A:81:ARG:CB	2.29	0.41
1:A:212:PHE:O	1:A:214:TRP:HE3	2.04	0.41
1:A:370:GLN:O	1:A:371:ALA:O	2.37	0.41
1:A:431:LEU:N	1:A:431:LEU:CD1	2.83	0.41
1:A:213:GLN:HG3	1:A:240:ASP:HB3	2.03	0.41
1:A:386:LYS:HE3	1:A:396:GLU:N	2.35	0.41
1:A:415:ILE:O	1:A:429:VAL:HA	2.21	0.41
1:A:431:LEU:C	1:A:433:THR:N	2.72	0.41
1:A:101:ILE:HB	1:A:216:ARG:NH1	2.36	0.41
1:A:326:THR:HG23	1:A:329:THR:H	1.85	0.41
1:A:523:THR:HG22	1:A:524:TYR:N	2.35	0.41
1:A:245:THR:HG21	1:A:248:ASN:OD1	2.21	0.40
1:A:275:LEU:HD23	1:A:275:LEU:HA	1.90	0.40
1:A:548:ILE:HA	1:A:548:ILE:HD12	1.64	0.40
1:A:160:PRO:HB2	1:A:161:PRO:HA	2.03	0.40
1:A:381:GLY:C	1:A:386:LYS:HB3	2.41	0.40
1:A:150:LEU:HG	1:A:525:SER:HB2	2.04	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	541/548 (99%)	503 (93%)	34 (6%)	4 (1%)	22 61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	CYS
1	A	371	ALA
1	A	55	GLU
1	A	579	ALA

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	474/476 (100%)	438 (92%)	36 (8%)	13 45

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	THR
1	A	47	ASN
1	A	56	ASN
1	A	67	ARG
1	A	72	ASN
1	A	80	ARG
1	A	85	ASN
1	A	96	MET
1	A	152	THR
1	A	177	LEU
1	A	183	MET
1	A	191	ARG
1	A	195	LEU
1	A	209	ARG
1	A	216	ARG
1	A	245	THR
1	A	257	THR
1	A	260	GLU
1	A	330	ILE
1	A	342	TYR
1	A	350	GLN
1	A	354	LYS
1	A	365	GLN
1	A	386	LYS
1	A	393	GLU
1	A	414	TRP
1	A	418	ILE
1	A	448	PHE
1	A	465	PRO
1	A	485	ASN

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Mol	Chain	Res	Type
1	A	490	CYS
1	A	493	ASN
1	A	520	ARG
1	A	548	ILE
1	A	574	GLU
1	A	578	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	56	ASN
1	A	78	ASN
1	A	85	ASN
1	A	147	ASN
1	A	159	GLN
1	A	180	ASN
1	A	234	HIS
1	A	242	GLN
1	A	282	ASN
1	A	310	GLN
1	A	323	ASN
1	A	365	GLN
1	A	383	GLN
1	A	384	HIS
1	A	416	GLN
1	A	428	ASN
1	A	443	ASN
1	A	458	ASN
1	A	466	ASN
1	A	468	GLN
1	A	485	ASN
1	A	497	GLN
1	A	546	ASN
1	A	560	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)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.