



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 03:02 AM EDT

PDB ID : 1K3V
Title : Porcine Parvovirus Capsid
Authors : Simpson, A.A.; Hebert, B.; Sullivan, G.M.; Parrish, C.R.; Zadori, Z.; Tijssen, P.; Rossmann, M.G.
Deposited on : 2001-10-04
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 ⓘ 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
Xtrriage (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) : 2.36.2

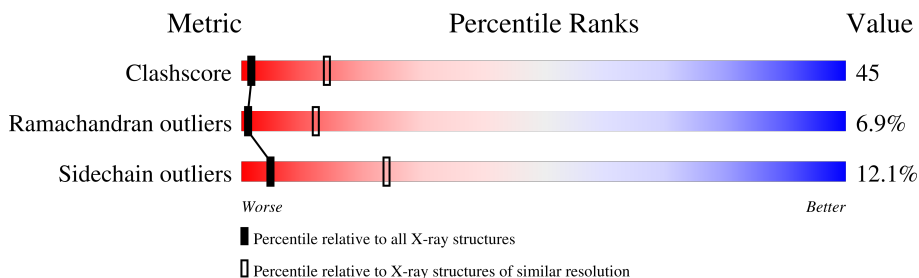
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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)

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	579	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4306 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 capsid protein VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	542	4306	2727	735	828	16	0	0	0

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	442.49Å 443.05Å 251.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.50	Depositor
% Data completeness (in resolution range)	31.4 (50.00-3.50)	Depositor
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.286 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4306	wwPDB-VP
Average B, all atoms (Å ²)	42.0	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	0.49	0/4432	0.77	1/6067 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	421	THR	N-CA-C	-5.04	97.38	111.00

There are no chirality outliers.

There are no planarity outliers.

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	4306	0	4137	377	0
All	All	4306	0	4137	377	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 45.

All (377) 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:246:THR:HG22	1:A:249:ASN:H	1.22	1.05
1:A:82:ARG:HE	1:A:236:THR:HG21	1.17	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:ALA:HB1	1:A:415:PRO:HD3	1.34	1.03
1:A:559:THR:HG22	1:A:561:ILE:H	1.24	1.02
1:A:193:GLU:HB3	1:A:206:THR:HG21	1.41	1.00
1:A:418:LEU:HD22	1:A:418:LEU:H	1.25	0.99
1:A:359:THR:HG21	1:A:402:CYS:HB2	1.47	0.95
1:A:406:PRO:HA	1:A:409:GLN:HG3	1.51	0.93
1:A:573:LEU:H	1:A:573:LEU:HD23	1.35	0.92
1:A:194:THR:HG22	1:A:195:LEU:H	1.34	0.92
1:A:453:LEU:HD12	1:A:454:ASN:H	1.34	0.91
1:A:101:ALA:HB3	1:A:216:ARG:NH1	1.85	0.91
1:A:544:GLN:O	1:A:545:GLN:HG2	1.71	0.91
1:A:79:THR:HG22	1:A:80:TYR:H	1.34	0.90
1:A:362:THR:HG21	1:A:405:ALA:HB2	1.55	0.88
1:A:174:MET:HE2	1:A:499:ALA:HA	1.55	0.87
1:A:441:MET:HE3	1:A:441:MET:H	1.39	0.86
1:A:48:ASN:HD22	1:A:67:SER:H	1.18	0.86
1:A:573:LEU:H	1:A:573:LEU:CD2	1.88	0.86
1:A:555:ASN:HA	1:A:565:ARG:HD2	1.58	0.85
1:A:261:GLU:HG2	1:A:262:PHE:N	1.92	0.85
1:A:321:ASN:HD22	1:A:321:ASN:H	1.21	0.85
1:A:159:SER:HB2	1:A:160:PRO:HD3	1.63	0.81
1:A:127:GLN:O	1:A:131:ASN:HB2	1.81	0.81
1:A:421:THR:HB	1:A:424:GLY:H	1.47	0.80
1:A:441:MET:H	1:A:441:MET:CE	1.93	0.80
1:A:414:ALA:HB1	1:A:415:PRO:CD	2.13	0.79
1:A:414:ALA:CB	1:A:415:PRO:HD3	2.11	0.79
1:A:212:LEU:HD23	1:A:213:SER:N	1.98	0.78
1:A:181:ASN:HD22	1:A:489:ASN:HD21	1.28	0.78
1:A:333:ALA:HB1	1:A:450:LEU:O	1.84	0.78
1:A:379:TYR:HE1	1:A:390:GLU:HA	1.49	0.76
1:A:292:LEU:HD12	1:A:292:LEU:H	1.51	0.76
1:A:159:SER:HB2	1:A:160:PRO:CD	2.15	0.75
1:A:559:THR:CG2	1:A:561:ILE:H	1.98	0.75
1:A:321:ASN:HD22	1:A:321:ASN:N	1.83	0.75
1:A:553:ILE:N	1:A:553:ILE:HD12	2.01	0.75
1:A:414:ALA:CB	1:A:415:PRO:CD	2.65	0.74
1:A:357:VAL:HG11	1:A:453:LEU:HD11	1.68	0.73
1:A:99:ASP:CG	1:A:216:ARG:HH12	1.91	0.73
1:A:215:ILE:HG13	1:A:237:GLY:HA2	1.71	0.73
1:A:183:LEU:HD12	1:A:495:PHE:CE2	2.24	0.72
1:A:82:ARG:NE	1:A:236:THR:HG21	2.00	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ASN:ND2	1:A:67:SER:H	1.88	0.72
1:A:82:ARG:HH11	1:A:82:ARG:HB3	1.54	0.71
1:A:413:GLN:CD	1:A:414:ALA:H	1.93	0.71
1:A:359:THR:HG21	1:A:403:GLY:H	1.55	0.71
1:A:359:THR:CG2	1:A:403:GLY:H	2.04	0.70
1:A:317:HIS:HB2	1:A:324:TYR:HE2	1.56	0.70
1:A:133:MET:HB2	1:A:276:LEU:HD12	1.72	0.70
1:A:559:THR:HG22	1:A:561:ILE:N	2.04	0.70
1:A:274:LEU:HD11	1:A:458:PRO:HG3	1.72	0.70
1:A:79:THR:HG22	1:A:80:TYR:N	2.07	0.69
1:A:111:LEU:HD23	1:A:112:ILE:N	2.06	0.69
1:A:43:THR:OG1	1:A:146:PHE:HB2	1.92	0.69
1:A:246:THR:HG22	1:A:249:ASN:N	2.03	0.69
1:A:129:ILE:O	1:A:133:MET:HG2	1.93	0.69
1:A:357:VAL:HG21	1:A:453:LEU:HD21	1.73	0.69
1:A:194:THR:HG22	1:A:195:LEU:N	2.08	0.69
1:A:390:GLU:HB3	1:A:391:LEU:HD23	1.73	0.68
1:A:440:PHE:CD2	1:A:441:MET:HE2	2.28	0.68
1:A:382:GLY:HA2	1:A:566:MET:HB2	1.76	0.68
1:A:132:ASN:HA	1:A:535:ARG:HD3	1.73	0.68
1:A:310:ALA:HB1	1:A:323:SER:HB2	1.75	0.68
1:A:121:PHE:HB3	1:A:125:ASP:HB2	1.76	0.67
1:A:418:LEU:O	1:A:419:GLU:HB2	1.93	0.67
1:A:427:LEU:HB3	1:A:428:PRO:HD2	1.77	0.66
1:A:456:THR:HG22	1:A:457:ALA:N	2.10	0.66
1:A:543:ILE:HG13	1:A:544:GLN:O	1.94	0.66
1:A:359:THR:HG21	1:A:402:CYS:CB	2.24	0.65
1:A:506:PHE:C	1:A:506:PHE:CD2	2.70	0.65
1:A:547:THR:OG1	1:A:548:THR:N	2.27	0.65
1:A:515:ARG:HG3	1:A:515:ARG:HH11	1.61	0.65
1:A:90:SER:OG	1:A:216:ARG:NH2	2.29	0.64
1:A:427:LEU:CB	1:A:428:PRO:HD2	2.27	0.64
1:A:453:LEU:CD1	1:A:454:ASN:H	2.09	0.64
1:A:48:ASN:ND2	1:A:66:ALA:HA	2.13	0.63
1:A:216:ARG:HG2	1:A:216:ARG:HH11	1.62	0.63
1:A:399:GLN:O	1:A:401:LYS:HD2	1.98	0.63
1:A:251:VAL:HG13	1:A:252:PRO:HD2	1.80	0.63
1:A:418:LEU:HD22	1:A:418:LEU:N	2.06	0.63
1:A:72:LEU:HD22	1:A:496:VAL:CG1	2.28	0.63
1:A:341:TYR:CD2	1:A:369:PRO:HB3	2.33	0.63
1:A:454:ASN:HD21	1:A:576:ARG:NH2	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:THR:HG23	1:A:515:ARG:HA	1.81	0.63
1:A:136:ILE:HG22	1:A:276:LEU:HD21	1.79	0.62
1:A:150:LEU:HD11	1:A:172:SER:C	2.19	0.62
1:A:216:ARG:HD2	1:A:217:ASN:H	1.65	0.62
1:A:310:ALA:O	1:A:312:THR:N	2.33	0.61
1:A:330:ILE:O	1:A:331:ARG:HD3	1.99	0.61
1:A:321:ASN:N	1:A:321:ASN:ND2	2.45	0.61
1:A:444:LEU:HD22	1:A:445:ASN:N	2.15	0.61
1:A:378:ASP:C	1:A:380:GLN:H	2.04	0.61
1:A:153:ILE:CG2	1:A:517:ILE:HB	2.31	0.61
1:A:456:THR:HG22	1:A:457:ALA:H	1.66	0.61
1:A:150:LEU:CD2	1:A:520:SER:HB2	2.31	0.60
1:A:317:HIS:HB2	1:A:324:TYR:CE2	2.34	0.60
1:A:377:MET:HG3	1:A:392:GLU:HB3	1.81	0.60
1:A:390:GLU:O	1:A:391:LEU:HG	2.02	0.60
1:A:453:LEU:HD12	1:A:454:ASN:N	2.12	0.60
1:A:553:ILE:HD12	1:A:553:ILE:H	1.66	0.60
1:A:277:THR:HG22	1:A:574:ILE:HB	1.83	0.60
1:A:87:ASN:HB2	1:A:89:GLU:OE1	2.02	0.59
1:A:571:SER:O	1:A:572:GLN:HB2	2.01	0.59
1:A:362:THR:OG1	1:A:363:GLN:N	2.34	0.59
1:A:191:ARG:O	1:A:193:GLU:HG3	2.03	0.59
1:A:515:ARG:N	1:A:515:ARG:HD3	2.18	0.59
1:A:96:MET:HE1	1:A:221:PRO:HB3	1.85	0.58
1:A:573:LEU:HD23	1:A:573:LEU:N	2.07	0.58
1:A:402:CYS:O	1:A:403:GLY:O	2.21	0.58
1:A:111:LEU:HD23	1:A:111:LEU:C	2.24	0.58
1:A:181:ASN:HD22	1:A:489:ASN:ND2	2.00	0.58
1:A:287:GLY:O	1:A:289:PRO:HD3	2.03	0.58
1:A:408:GLN:HE21	1:A:408:GLN:C	2.06	0.57
1:A:377:MET:CG	1:A:392:GLU:HB3	2.33	0.57
1:A:274:LEU:HD23	1:A:275:LYS:O	2.04	0.57
1:A:43:THR:H	1:A:147:ASN:ND2	2.02	0.57
1:A:72:LEU:HD22	1:A:496:VAL:HG12	1.87	0.57
1:A:364:TYR:HD1	1:A:364:TYR:N	2.03	0.57
1:A:336:GLY:O	1:A:337:TYR:HB3	2.05	0.57
1:A:469:GLU:OE1	1:A:470:LEU:N	2.37	0.56
1:A:550:ALA:O	1:A:553:ILE:HD11	2.06	0.56
1:A:359:THR:HG21	1:A:403:GLY:N	2.20	0.56
1:A:92:VAL:HG12	1:A:93:ALA:N	2.21	0.56
1:A:394:TYR:CZ	1:A:568:PRO:HG3	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ARG:NH1	1:A:196:GLY:O	2.37	0.56
1:A:394:TYR:CE2	1:A:568:PRO:HG3	2.40	0.56
1:A:418:LEU:O	1:A:419:GLU:CB	2.53	0.56
1:A:573:LEU:CD2	1:A:573:LEU:N	2.62	0.56
1:A:341:TYR:HD1	1:A:341:TYR:H	1.54	0.56
1:A:246:THR:CG2	1:A:249:ASN:H	2.08	0.56
1:A:321:ASN:H	1:A:321:ASN:ND2	1.98	0.56
1:A:129:ILE:HG23	1:A:133:MET:HG3	1.88	0.55
1:A:200:TRP:CZ2	1:A:564:ILE:HD13	2.41	0.55
1:A:364:TYR:N	1:A:364:TYR:CD1	2.75	0.55
1:A:101:ALA:HB3	1:A:216:ARG:HH11	1.71	0.55
1:A:75:PRO:HG2	1:A:497:LYS:HG3	1.89	0.55
1:A:309:ALA:O	1:A:310:ALA:O	2.25	0.55
1:A:223:TYR:O	1:A:225:GLY:N	2.40	0.54
1:A:159:SER:CB	1:A:160:PRO:CD	2.83	0.54
1:A:246:THR:HB	1:A:249:ASN:HB2	1.88	0.54
1:A:298:THR:HB	1:A:303:HIS:ND1	2.23	0.54
1:A:39:VAL:HG13	1:A:40:GLY:H	1.72	0.54
1:A:274:LEU:HD23	1:A:275:LYS:N	2.23	0.54
1:A:118:GLY:CA	1:A:461:PRO:HB2	2.38	0.54
1:A:150:LEU:HD23	1:A:520:SER:HB2	1.90	0.54
1:A:421:THR:HB	1:A:424:GLY:N	2.21	0.53
1:A:404:ARG:HG3	1:A:404:ARG:HH11	1.72	0.53
1:A:506:PHE:CD2	1:A:507:ASN:N	2.75	0.53
1:A:553:ILE:N	1:A:553:ILE:CD1	2.66	0.53
1:A:353:LEU:HD23	1:A:354:THR:C	2.29	0.53
1:A:378:ASP:OD2	1:A:379:TYR:N	2.42	0.53
1:A:553:ILE:H	1:A:553:ILE:CD1	2.17	0.53
1:A:97:VAL:HG13	1:A:344:PHE:CE2	2.44	0.53
1:A:216:ARG:HD2	1:A:233:SER:O	2.09	0.53
1:A:506:PHE:CG	1:A:507:ASN:N	2.75	0.53
1:A:212:LEU:HD23	1:A:213:SER:H	1.70	0.52
1:A:426:LEU:HD23	1:A:440:PHE:CD2	2.44	0.52
1:A:153:ILE:HG23	1:A:153:ILE:O	2.10	0.52
1:A:296:PRO:HG3	1:A:304:PRO:O	2.10	0.52
1:A:413:GLN:OE1	1:A:414:ALA:N	2.36	0.52
1:A:48:ASN:ND2	1:A:68:ARG:HH21	2.07	0.52
1:A:185:TYR:HA	1:A:493:GLN:NE2	2.24	0.52
1:A:375:PHE:HB2	1:A:394:TYR:CE2	2.44	0.52
1:A:215:ILE:O	1:A:215:ILE:HG22	2.10	0.52
1:A:359:THR:HG22	1:A:360:ALA:N	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:PHE:CG	1:A:441:MET:HE2	2.44	0.52
1:A:255:LEU:O	1:A:256:LEU:HD23	2.10	0.52
1:A:454:ASN:HD21	1:A:576:ARG:HH22	1.57	0.52
1:A:544:GLN:NE2	1:A:573:LEU:HB2	2.25	0.52
1:A:96:MET:HE1	1:A:221:PRO:CB	2.40	0.52
1:A:518:THR:HG22	1:A:519:TYR:N	2.25	0.52
1:A:216:ARG:HD2	1:A:217:ASN:N	2.25	0.52
1:A:60:VAL:HG22	1:A:532:ALA:O	2.10	0.51
1:A:174:MET:HB2	1:A:497:LYS:O	2.11	0.51
1:A:130:SER:HB2	1:A:573:LEU:HD21	1.92	0.51
1:A:186:THR:H	1:A:493:GLN:HE22	1.57	0.51
1:A:339:THR:HB	1:A:356:ILE:HG23	1.93	0.51
1:A:115:ASN:ND2	1:A:464:GLN:CG	2.73	0.51
1:A:213:SER:OG	1:A:237:GLY:HA3	2.11	0.51
1:A:235:GLN:O	1:A:236:THR:C	2.50	0.51
1:A:236:THR:O	1:A:237:GLY:O	2.29	0.51
1:A:294:THR:HB	1:A:306:THR:H	1.75	0.51
1:A:406:PRO:O	1:A:408:GLN:N	2.44	0.50
1:A:489:ASN:HD22	1:A:490:PRO:HD2	1.76	0.50
1:A:74:MET:HE1	1:A:517:ILE:HA	1.92	0.50
1:A:416:LEU:O	1:A:417:ASN:CB	2.60	0.50
1:A:83:ILE:HG22	1:A:84:HIS:O	2.11	0.50
1:A:178:ASP:OD2	1:A:181:ASN:HA	2.11	0.50
1:A:276:LEU:O	1:A:572:GLN:HA	2.11	0.50
1:A:505:ASP:O	1:A:506:PHE:O	2.30	0.50
1:A:115:ASN:HD21	1:A:464:GLN:HG2	1.77	0.50
1:A:364:TYR:O	1:A:365:ASN:C	2.49	0.50
1:A:565:ARG:HD3	1:A:567:PHE:CE1	2.47	0.50
1:A:39:VAL:HG13	1:A:40:GLY:N	2.27	0.50
1:A:94:GLY:N	1:A:222:THR:OG1	2.39	0.50
1:A:158:THR:O	1:A:158:THR:HG23	2.11	0.49
1:A:121:PHE:HB3	1:A:125:ASP:CB	2.42	0.49
1:A:55:LEU:N	1:A:55:LEU:HD12	2.27	0.49
1:A:379:TYR:CE1	1:A:390:GLU:HG2	2.48	0.49
1:A:113:ASP:O	1:A:195:LEU:HD13	2.11	0.49
1:A:515:ARG:HG3	1:A:515:ARG:NH1	2.27	0.49
1:A:43:THR:HB	1:A:261:GLU:HB2	1.95	0.49
1:A:82:ARG:HD2	1:A:212:LEU:HD13	1.95	0.49
1:A:180:ASN:HD22	1:A:180:ASN:N	2.09	0.49
1:A:216:ARG:NH1	1:A:216:ARG:HG2	2.27	0.49
1:A:407:LYS:O	1:A:408:GLN:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:PHE:CD1	1:A:440:PHE:C	2.85	0.49
1:A:79:THR:CG2	1:A:80:TYR:H	2.15	0.49
1:A:346:TYR:HD1	1:A:351:PRO:HB3	1.76	0.49
1:A:297:THR:O	1:A:297:THR:HG22	2.12	0.49
1:A:310:ALA:O	1:A:311:ASN:C	2.51	0.49
1:A:111:LEU:HD21	1:A:113:ASP:HB2	1.95	0.49
1:A:392:GLU:HG2	1:A:567:PHE:HE2	1.78	0.48
1:A:62:ILE:HD11	1:A:133:MET:CE	2.43	0.48
1:A:158:THR:O	1:A:160:PRO:HD2	2.13	0.48
1:A:303:HIS:N	1:A:303:HIS:CD2	2.78	0.48
1:A:153:ILE:HG22	1:A:517:ILE:HB	1.96	0.48
1:A:378:ASP:C	1:A:380:GLN:N	2.67	0.48
1:A:130:SER:HB2	1:A:573:LEU:CD2	2.43	0.48
1:A:325:THR:HG22	1:A:326:GLU:N	2.28	0.48
1:A:102:HIS:HA	1:A:214:CYS:SG	2.53	0.48
1:A:115:ASN:ND2	1:A:464:GLN:HG3	2.29	0.48
1:A:85:VAL:O	1:A:101:ALA:HA	2.13	0.48
1:A:197:PHE:HB3	1:A:566:MET:CE	2.44	0.48
1:A:416:LEU:HB3	1:A:417:ASN:H	1.50	0.48
1:A:528:LEU:HG	1:A:530:PHE:CE2	2.49	0.48
1:A:392:GLU:HG3	1:A:393:ARG:N	2.29	0.48
1:A:549:THR:C	1:A:551:GLU:H	2.17	0.48
1:A:559:THR:HB	1:A:563:GLY:H	1.78	0.48
1:A:53:GLN:HB2	1:A:61:ARG:HB3	1.96	0.47
1:A:353:LEU:HD23	1:A:353:LEU:C	2.35	0.47
1:A:456:THR:CG2	1:A:457:ALA:N	2.76	0.47
1:A:360:ALA:HB2	1:A:398:PRO:O	2.14	0.47
1:A:48:ASN:HD21	1:A:68:ARG:HH21	1.60	0.47
1:A:212:LEU:HD21	1:A:242:ILE:HG13	1.97	0.47
1:A:256:LEU:HD22	1:A:260:ASP:HB3	1.96	0.47
1:A:384:LEU:HG	1:A:565:ARG:HG2	1.97	0.47
1:A:298:THR:HB	1:A:303:HIS:CE1	2.49	0.47
1:A:87:ASN:OD1	1:A:90:SER:HB2	2.15	0.47
1:A:347:SER:O	1:A:349:GLY:N	2.48	0.47
1:A:468:LYS:HA	1:A:490:PRO:HG2	1.96	0.47
1:A:557:ILE:HG22	1:A:558:PRO:O	2.15	0.47
1:A:209:ARG:O	1:A:209:ARG:HG2	2.15	0.46
1:A:223:TYR:CZ	1:A:226:GLN:HB3	2.50	0.46
1:A:200:TRP:HZ2	1:A:564:ILE:HD13	1.79	0.46
1:A:274:LEU:CD1	1:A:483:PRO:HB2	2.44	0.46
1:A:506:PHE:C	1:A:506:PHE:HD2	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:PHE:HA	1:A:461:PRO:HA	1.75	0.46
1:A:48:ASN:HD21	1:A:68:ARG:NH2	2.13	0.46
1:A:141:PHE:CZ	1:A:143:GLN:CG	2.99	0.46
1:A:383:HIS:O	1:A:384:LEU:C	2.54	0.46
1:A:416:LEU:O	1:A:417:ASN:HB3	2.16	0.46
1:A:418:LEU:N	1:A:418:LEU:HD13	2.29	0.46
1:A:443:THR:O	1:A:443:THR:CG2	2.64	0.46
1:A:466:TRP:HA	1:A:484:PHE:HB2	1.97	0.46
1:A:274:LEU:HD23	1:A:274:LEU:C	2.36	0.46
1:A:197:PHE:HB3	1:A:566:MET:HE2	1.97	0.46
1:A:74:MET:CE	1:A:517:ILE:HA	2.44	0.46
1:A:74:MET:HB2	1:A:518:THR:O	2.16	0.46
1:A:136:ILE:HG12	1:A:137:ASN:N	2.29	0.46
1:A:173:LEU:HD12	1:A:174:MET:N	2.31	0.46
1:A:428:PRO:HA	1:A:441:MET:HE1	1.97	0.46
1:A:68:ARG:NH2	1:A:199:PRO:HG3	2.30	0.46
1:A:94:GLY:C	1:A:96:MET:H	2.19	0.46
1:A:334:GLN:HE22	1:A:446:THR:HB	1.80	0.46
1:A:440:PHE:N	1:A:441:MET:HE3	2.31	0.46
1:A:150:LEU:HD12	1:A:171:ALA:C	2.36	0.45
1:A:359:THR:CG2	1:A:360:ALA:N	2.78	0.45
1:A:94:GLY:O	1:A:96:MET:N	2.49	0.45
1:A:329:ALA:HB3	1:A:331:ARG:NH1	2.32	0.45
1:A:92:VAL:CG1	1:A:93:ALA:N	2.80	0.45
1:A:489:ASN:HD22	1:A:490:PRO:CD	2.29	0.45
1:A:93:ALA:HA	1:A:222:THR:OG1	2.17	0.45
1:A:274:LEU:HD12	1:A:483:PRO:HB2	1.98	0.45
1:A:82:ARG:HB3	1:A:82:ARG:NH1	2.28	0.45
1:A:200:TRP:HE1	1:A:564:ILE:HD11	1.80	0.45
1:A:379:TYR:CE1	1:A:390:GLU:HA	2.40	0.45
1:A:56:GLY:O	1:A:58:GLY:N	2.50	0.45
1:A:339:THR:O	1:A:340:PRO:C	2.55	0.45
1:A:82:ARG:HH11	1:A:82:ARG:CB	2.28	0.44
1:A:280:TRP:CG	1:A:281:GLN:N	2.85	0.44
1:A:367:ASP:O	1:A:370:ASN:N	2.44	0.44
1:A:368:GLU:N	1:A:369:PRO:HD2	2.32	0.44
1:A:378:ASP:O	1:A:380:GLN:N	2.50	0.44
1:A:576:ARG:HG2	1:A:577:LYS:O	2.17	0.44
1:A:310:ALA:HB1	1:A:323:SER:CB	2.45	0.44
1:A:302:GLN:HB2	1:A:303:HIS:CD2	2.52	0.44
1:A:188:ALA:C	1:A:190:PRO:HD2	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:GLN:HE21	1:A:409:GLN:HB3	1.52	0.44
1:A:138:LEU:HD12	1:A:138:LEU:HA	1.81	0.44
1:A:48:ASN:ND2	1:A:67:SER:N	2.62	0.44
1:A:114:ALA:HB1	1:A:119:VAL:HG11	2.00	0.44
1:A:274:LEU:CD2	1:A:275:LYS:O	2.66	0.44
1:A:393:ARG:CG	1:A:394:TYR:H	2.31	0.44
1:A:97:VAL:HG13	1:A:344:PHE:CZ	2.52	0.43
1:A:279:SER:HB2	1:A:578:LEU:HD12	2.00	0.43
1:A:367:ASP:C	1:A:369:PRO:HD2	2.39	0.43
1:A:68:ARG:HD3	1:A:196:GLY:O	2.18	0.43
1:A:300:GLY:C	1:A:302:GLN:H	2.22	0.43
1:A:392:GLU:HG3	1:A:393:ARG:H	1.84	0.43
1:A:405:ALA:O	1:A:408:GLN:HB2	2.18	0.43
1:A:101:ALA:HB1	1:A:234:ILE:HD12	1.99	0.43
1:A:390:GLU:C	1:A:391:LEU:HG	2.38	0.43
1:A:559:THR:C	1:A:561:ILE:H	2.21	0.43
1:A:141:PHE:CZ	1:A:143:GLN:HG2	2.53	0.43
1:A:550:ALA:C	1:A:553:ILE:HD11	2.38	0.43
1:A:558:PRO:HA	1:A:563:GLY:O	2.18	0.43
1:A:261:GLU:HG2	1:A:262:PHE:H	1.77	0.43
1:A:565:ARG:HD3	1:A:567:PHE:HE1	1.83	0.43
1:A:353:LEU:HD23	1:A:354:THR:N	2.33	0.43
1:A:56:GLY:C	1:A:58:GLY:H	2.22	0.43
1:A:180:ASN:N	1:A:180:ASN:ND2	2.66	0.43
1:A:267:TYR:CD2	1:A:491:PRO:HB3	2.54	0.43
1:A:384:LEU:HD21	1:A:565:ARG:NH1	2.34	0.43
1:A:455:ASN:OD1	1:A:456:THR:N	2.51	0.43
1:A:360:ALA:N	1:A:398:PRO:HG2	2.34	0.42
1:A:200:TRP:HE1	1:A:564:ILE:CD1	2.32	0.42
1:A:274:LEU:HD22	1:A:276:LEU:HD23	2.01	0.42
1:A:282:THR:O	1:A:285:SER:N	2.50	0.42
1:A:505:ASP:O	1:A:506:PHE:HD2	2.02	0.42
1:A:517:ILE:H	1:A:517:ILE:HG13	1.69	0.42
1:A:46:PHE:CD1	1:A:46:PHE:C	2.92	0.42
1:A:101:ALA:O	1:A:102:HIS:HB3	2.19	0.42
1:A:258:THR:HG23	1:A:259:GLY:N	2.34	0.42
1:A:386:THR:O	1:A:387:SER:C	2.58	0.42
1:A:549:THR:HG23	1:A:552:ASN:ND2	2.34	0.42
1:A:418:LEU:H	1:A:418:LEU:CD2	2.01	0.42
1:A:456:THR:CG2	1:A:457:ALA:H	2.31	0.42
1:A:391:LEU:HD23	1:A:391:LEU:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:THR:HG22	1:A:525:LYS:NZ	2.35	0.42
1:A:48:ASN:HD22	1:A:67:SER:N	1.99	0.42
1:A:278:HIS:HB2	1:A:400:SER:HA	2.01	0.42
1:A:502:LEU:HD13	1:A:507:ASN:ND2	2.35	0.42
1:A:116:ALA:HB3	1:A:194:THR:HG21	2.02	0.42
1:A:267:TYR:CE2	1:A:491:PRO:HD3	2.55	0.42
1:A:338:ASN:HB2	1:A:444:LEU:HD13	2.02	0.42
1:A:425:THR:HG22	1:A:427:LEU:CD1	2.50	0.42
1:A:482:ALA:HB1	1:A:483:PRO:HD2	2.01	0.42
1:A:345:GLU:O	1:A:351:PRO:HA	2.21	0.41
1:A:111:LEU:CD2	1:A:113:ASP:HB2	2.50	0.41
1:A:156:SER:C	1:A:158:THR:H	2.23	0.41
1:A:109:TRP:CD1	1:A:247:ILE:HG13	2.55	0.41
1:A:138:LEU:HD13	1:A:530:PHE:CE1	2.55	0.41
1:A:280:TRP:O	1:A:281:GLN:C	2.58	0.41
1:A:86:LEU:HD23	1:A:86:LEU:HA	1.90	0.41
1:A:559:THR:HG23	1:A:560:ASN:N	2.34	0.41
1:A:96:MET:H	1:A:96:MET:HG3	1.69	0.41
1:A:453:LEU:CG	1:A:454:ASN:N	2.84	0.41
1:A:138:LEU:HG	1:A:269:PHE:CD1	2.56	0.41
1:A:346:TYR:CE1	1:A:351:PRO:HD3	2.55	0.41
1:A:394:TYR:CD2	1:A:568:PRO:HG3	2.56	0.41
1:A:489:ASN:ND2	1:A:490:PRO:HD2	2.36	0.41
1:A:549:THR:C	1:A:551:GLU:N	2.72	0.41
1:A:498:ILE:CD1	1:A:519:TYR:HA	2.50	0.41
1:A:43:THR:HG21	1:A:260:ASP:O	2.21	0.41
1:A:115:ASN:HD21	1:A:464:GLN:CG	2.33	0.41
1:A:138:LEU:HG	1:A:269:PHE:CE1	2.56	0.41
1:A:189:ALA:N	1:A:190:PRO:HD2	2.36	0.41
1:A:238:LEU:HD23	1:A:238:LEU:HA	1.95	0.41
1:A:246:THR:CG2	1:A:248:GLU:HB2	2.51	0.41
1:A:300:GLY:C	1:A:302:GLN:N	2.74	0.41
1:A:394:TYR:CE1	1:A:568:PRO:HG3	2.55	0.41
1:A:421:THR:O	1:A:422:ASN:C	2.57	0.41
1:A:275:LYS:HD2	1:A:576:ARG:NH1	2.36	0.41
1:A:317:HIS:CD2	1:A:319:THR:OG1	2.74	0.41
1:A:219:ASN:HA	1:A:220:PRO:HA	1.72	0.40
1:A:382:GLY:O	1:A:383:HIS:HB3	2.21	0.40
1:A:359:THR:HG22	1:A:403:GLY:H	1.82	0.40
1:A:366:ASP:HB3	1:A:369:PRO:CG	2.51	0.40
1:A:513:GLN:H	1:A:513:GLN:HG3	1.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:PHE:HA	1:A:527:THR:O	2.21	0.40
1:A:183:LEU:HD12	1:A:495:PHE:CZ	2.54	0.40
1:A:427:LEU:CB	1:A:428:PRO:CD	2.99	0.40
1:A:577:LYS:HE3	1:A:577:LYS:HB2	1.68	0.40
1:A:364:TYR:O	1:A:366:ASP:N	2.54	0.40
1:A:468:LYS:HA	1:A:490:PRO:CG	2.51	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	540/579 (93%)	425 (79%)	78 (14%)	37 (7%)	1 12

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	SER
1	A	224	THR
1	A	226	GLN
1	A	237	GLY
1	A	310	ALA
1	A	311	ASN
1	A	348	ASN
1	A	387	SER
1	A	403	GLY
1	A	408	GLN
1	A	414	ALA
1	A	419	GLU
1	A	420	ASN
1	A	506	PHE
1	A	511	PRO

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Mol	Chain	Res	Type
1	A	57	GLU
1	A	78	GLU
1	A	95	GLN
1	A	365	ASN
1	A	391	LEU
1	A	157	ALA
1	A	379	TYR
1	A	383	HIS
1	A	384	LEU
1	A	417	ASN
1	A	456	THR
1	A	322	ASN
1	A	337	TYR
1	A	367	ASP
1	A	394	TYR
1	A	502	LEU
1	A	102	HIS
1	A	161	PRO
1	A	312	THR
1	A	340	PRO
1	A	508	ALA
1	A	377	MET

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	480/501 (96%)	422 (88%)	58 (12%)	5 24

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	THR
1	A	73	ASN
1	A	105	MET
1	A	131	ASN

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Mol	Chain	Res	Type
1	A	138	LEU
1	A	152	THR
1	A	159	SER
1	A	172	SER
1	A	209	ARG
1	A	220	PRO
1	A	236	THR
1	A	242	ILE
1	A	247	ILE
1	A	282	THR
1	A	285	SER
1	A	292	LEU
1	A	293	LEU
1	A	298	THR
1	A	304	PRO
1	A	311	ASN
1	A	312	THR
1	A	314	LYS
1	A	317	HIS
1	A	321	ASN
1	A	339	THR
1	A	341	TYR
1	A	356	ILE
1	A	362	THR
1	A	363	GLN
1	A	364	TYR
1	A	365	ASN
1	A	376	THR
1	A	385	THR
1	A	387	SER
1	A	391	LEU
1	A	393	ARG
1	A	394	TYR
1	A	408	GLN
1	A	409	GLN
1	A	413	GLN
1	A	416	LEU
1	A	418	LEU
1	A	440	PHE
1	A	441	MET
1	A	444	LEU
1	A	454	ASN

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Mol	Chain	Res	Type
1	A	461	PRO
1	A	506	PHE
1	A	512	GLN
1	A	513	GLN
1	A	515	ARG
1	A	531	THR
1	A	538	ASN
1	A	553	ILE
1	A	559	THR
1	A	566	MET
1	A	573	LEU
1	A	578	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	48	ASN
1	A	49	GLN
1	A	73	ASN
1	A	147	ASN
1	A	180	ASN
1	A	303	HIS
1	A	317	HIS
1	A	321	ASN
1	A	380	GLN
1	A	408	GLN
1	A	409	GLN
1	A	412	GLN
1	A	454	ASN
1	A	462	ASN
1	A	489	ASN
1	A	493	GLN
1	A	513	GLN
1	A	541	ASN
1	A	544	GLN
1	A	555	ASN

5.3.3 RNA

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

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.