



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 02:03 AM GMT

PDB ID : 1C8H  
Title : CANINE PARVOVIRUS STRAIN D EMPTY CAPSID STRUCTURE AT PH  
5.5  
Authors : Rossmann, M.G.; Simpson, A.A.  
Deposited on : 2000-05-05  
Resolution : 3.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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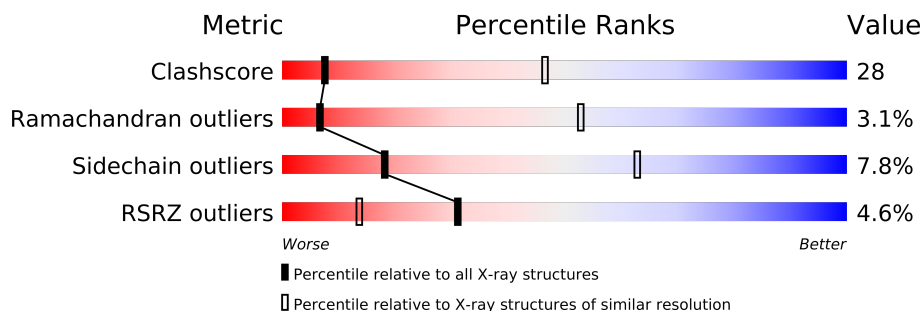
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	584	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4321 atoms, of which 0 are hydrogen and 0 are deuterium.

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 CANINE PARVOVIRUS CAPSID.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	544	4319	2745	737	821	16	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	386	GLN	LYS	ENGINEERED	GB 758434

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	254.49Å 253.60Å 452.04Å 77.48° 74.91° 69.27°	Depositor
Resolution (Å)	9.00 – 3.50 20.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (9.00-3.50) 57.2 (20.00-3.50)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1457.89 (at 3.52Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, $R_{free}$	0.260 , (Not available) 0.323 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	30.3	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 91.8	EDS
Estimated twinning fraction	0.169 for -k,-h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.35$ , $\langle L^2 \rangle = 0.17$	Xtriage
Outliers	0 of 810511 reflections	Xtriage
$F_o, F_c$ correlation	0.08	EDS
Total number of atoms	4321	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.54	0/4448	0.77	2/6086 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	TRP	N-CA-C	-5.17	97.03	111.00
1	A	168	ASP	N-CA-C	-5.15	97.10	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4319	0	4118	233	0
2	A	2	0	0	0	0
All	All	4321	0	4118	233	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 28.

All (233) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:366:THR:HA	1:A:370:GLN:HB2	1.24	1.09
1:A:360:GLY:HA2	1:A:374:GLY:HA3	1.36	1.07
1:A:155:GLU:HB3	1:A:160:PRO:HA	1.44	0.99
1:A:160:PRO:HB2	1:A:161:PRO:CD	1.95	0.95
1:A:160:PRO:HB2	1:A:161:PRO:HD3	1.47	0.92
1:A:554:ASN:H	1:A:557:ASN:HD21	0.98	0.92
1:A:322:THR:HG21	1:A:420:PHE:HD2	1.38	0.89
1:A:154:SER:HB2	1:A:164:VAL:HG22	1.56	0.88
1:A:361:ARG:HG2	1:A:362:GLY:H	1.39	0.88
1:A:422:LEU:HD23	1:A:422:LEU:H	1.39	0.87
1:A:366:THR:HA	1:A:370:GLN:CB	2.05	0.87
1:A:349:THR:HG22	1:A:350:GLN:HG3	1.56	0.85
1:A:554:ASN:H	1:A:557:ASN:ND2	1.74	0.85
1:A:557:ASN:HD22	1:A:558:GLN:N	1.76	0.81
1:A:213:GLN:HG3	1:A:240:ASP:HB2	1.62	0.80
1:A:193:GLU:HB3	1:A:206:THR:HG21	1.65	0.78
1:A:554:ASN:N	1:A:557:ASN:HD21	1.79	0.78
1:A:52:LYS:HG2	1:A:54:LEU:HD21	1.66	0.78
1:A:139:VAL:HB	1:A:534:VAL:O	1.83	0.77
1:A:96:MET:HG2	1:A:220:PRO:HA	1.67	0.76
1:A:155:GLU:HB3	1:A:160:PRO:CA	2.16	0.76
1:A:560:ASN:HB3	1:A:572:VAL:HG21	1.66	0.76
1:A:410:PRO:HA	1:A:413:ASP:OD2	1.87	0.75
1:A:360:GLY:HA2	1:A:374:GLY:CA	2.16	0.75
1:A:38:VAL:HG21	1:A:169:LEU:HD13	1.67	0.74
1:A:560:ASN:HB3	1:A:572:VAL:CG2	2.18	0.74
1:A:557:ASN:HD22	1:A:558:GLN:H	1.36	0.73
1:A:322:THR:HG21	1:A:420:PHE:CD2	2.22	0.72
1:A:154:SER:O	1:A:163:LYS:HA	1.90	0.71
1:A:322:THR:CG2	1:A:420:PHE:HD2	2.04	0.71
1:A:180:ASN:O	1:A:181:ASN:HB2	1.90	0.69
1:A:408:ARG:HH11	1:A:408:ARG:HG3	1.56	0.69
1:A:219:ILE:HG23	1:A:220:PRO:HD2	1.74	0.69
1:A:221:SER:HB2	1:A:225:THR:HG21	1.74	0.69
1:A:67:ARG:HH11	1:A:67:ARG:HG2	1.57	0.68
1:A:361:ARG:HG2	1:A:362:GLY:N	2.10	0.67
1:A:316:VAL:O	1:A:330:ILE:HD12	1.95	0.67
1:A:43:GLY:HA3	1:A:146:PHE:CD2	2.31	0.66
1:A:160:PRO:CB	1:A:161:PRO:CD	2.71	0.66
1:A:366:THR:O	1:A:370:GLN:HG2	1.96	0.66
1:A:366:THR:CA	1:A:370:GLN:HB2	2.15	0.66
1:A:69:VAL:HG13	1:A:205:PRO:HD3	1.78	0.65
1:A:94:GLY:HA2	1:A:221:SER:O	1.98	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:92:VAL:O	1:A:93:ASN:HB2	1.97	0.64
1:A:213:GLN:HG3	1:A:240:ASP:CB	2.28	0.63
1:A:68:LEU:O	1:A:68:LEU:HG	1.98	0.63
1:A:330:ILE:HG13	1:A:331:MET:N	2.12	0.63
1:A:339:SER:O	1:A:449:ASN:HA	1.98	0.63
1:A:99:ASP:OD1	1:A:216:ARG:NH2	2.30	0.62
1:A:58:TRP:CE3	1:A:536:LYS:HE3	2.34	0.62
1:A:47:ASN:OD1	1:A:66:SER:N	2.29	0.61
1:A:154:SER:HB2	1:A:164:VAL:CG2	2.29	0.61
1:A:67:ARG:HG2	1:A:67:ARG:NH1	2.16	0.61
1:A:464:TYR:CE2	1:A:465:PRO:HB3	2.35	0.61
1:A:70:HIS:O	1:A:204:ILE:HG22	2.01	0.61
1:A:422:LEU:HA	1:A:423:PRO:C	2.21	0.60
1:A:282:ASN:HA	1:A:285:LEU:HD12	1.82	0.60
1:A:87:MET:HG3	1:A:231:ASN:ND2	2.17	0.59
1:A:79:TYR:CE2	1:A:107:THR:HG22	2.37	0.59
1:A:460:VAL:HG11	1:A:484:VAL:HA	1.83	0.59
1:A:55:GLU:O	1:A:56:ASN:HB2	2.01	0.59
1:A:422:LEU:CD2	1:A:422:LEU:H	2.13	0.59
1:A:422:LEU:HD23	1:A:422:LEU:N	2.15	0.59
1:A:38:VAL:HG12	1:A:39:GLY:N	2.18	0.59
1:A:354:LYS:HD2	1:A:355:THR:N	2.17	0.59
1:A:193:GLU:CB	1:A:206:THR:HG21	2.31	0.59
1:A:282:ASN:OD1	1:A:335:GLU:HA	2.03	0.59
1:A:160:PRO:C	1:A:162:THR:N	2.56	0.58
1:A:53:PHE:CD1	1:A:59:VAL:HG22	2.38	0.58
1:A:115:ASN:OD1	1:A:468:GLN:HG2	2.04	0.58
1:A:317:THR:HG22	1:A:330:ILE:HA	1.84	0.58
1:A:560:ASN:CB	1:A:572:VAL:HG21	2.34	0.58
1:A:354:LYS:HD2	1:A:355:THR:H	1.68	0.58
1:A:47:ASN:ND2	1:A:199:PRO:HB3	2.19	0.58
1:A:160:PRO:C	1:A:162:THR:H	2.05	0.58
1:A:361:ARG:HG2	1:A:366:THR:HG21	1.86	0.58
1:A:68:LEU:CG	1:A:68:LEU:O	2.51	0.57
1:A:281:THR:O	1:A:283:ARG:N	2.37	0.57
1:A:49:THR:C	1:A:50:GLU:HG3	2.24	0.57
1:A:357:ILE:HG22	1:A:359:ALA:H	1.70	0.57
1:A:348:SER:O	1:A:350:GLN:N	2.38	0.56
1:A:465:PRO:HD3	1:A:573:TYR:HA	1.87	0.56
1:A:69:VAL:HB	1:A:527:PHE:CE1	2.40	0.56
1:A:536:LYS:O	1:A:536:LYS:HG2	2.04	0.56
1:A:408:ARG:HG3	1:A:408:ARG:NH1	2.20	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:346:GLU:HG3	1:A:355:THR:OG1	2.06	0.56
1:A:197:PHE:CE2	1:A:384:HIS:HB3	2.40	0.56
1:A:295:PRO:HD3	1:A:304:GLY:CA	2.36	0.56
1:A:59:VAL:HG12	1:A:60:GLU:N	2.22	0.55
1:A:197:PHE:CE2	1:A:465:PRO:O	2.59	0.55
1:A:193:GLU:CG	1:A:206:THR:HG21	2.35	0.55
1:A:398:PHE:HE1	1:A:400:TYR:HB2	1.71	0.55
1:A:409:TYR:CE2	1:A:411:GLU:HB2	2.42	0.55
1:A:457:LEU:N	1:A:457:LEU:HD23	2.22	0.55
1:A:52:LYS:HD3	1:A:60:GLU:OE2	2.07	0.55
1:A:38:VAL:CG2	1:A:169:LEU:HD13	2.35	0.55
1:A:107:THR:HG21	1:A:208:TRP:CZ3	2.41	0.54
1:A:465:PRO:HD2	1:A:466:ASN:ND2	2.22	0.54
1:A:361:ARG:NE	1:A:366:THR:HG22	2.22	0.54
1:A:387:LYS:O	1:A:390:THR:HB	2.07	0.54
1:A:361:ARG:HE	1:A:366:THR:HG22	1.71	0.54
1:A:160:PRO:O	1:A:162:THR:N	2.41	0.54
1:A:557:ASN:ND2	1:A:557:ASN:H	2.05	0.54
1:A:330:ILE:HG13	1:A:331:MET:H	1.71	0.54
1:A:261:PHE:CD1	1:A:261:PHE:C	2.81	0.54
1:A:557:ASN:O	1:A:559:PHE:N	2.41	0.53
1:A:361:ARG:CG	1:A:362:GLY:N	2.71	0.53
1:A:219:ILE:CG2	1:A:220:PRO:HD2	2.38	0.53
1:A:340:ALA:HB3	1:A:357:ILE:HD12	1.89	0.53
1:A:396:GLU:HA	1:A:396:GLU:OE1	2.07	0.53
1:A:47:ASN:OD1	1:A:65:SER:HA	2.08	0.53
1:A:363:GLY:HA3	1:A:365:GLN:NE2	2.23	0.53
1:A:317:THR:HG21	1:A:329:THR:HG22	1.90	0.53
1:A:59:VAL:HG21	1:A:133:MET:HE2	1.92	0.52
1:A:219:ILE:HG12	1:A:230:THR:OG1	2.08	0.52
1:A:557:ASN:ND2	1:A:558:GLN:N	2.53	0.52
1:A:422:LEU:N	1:A:422:LEU:CD2	2.72	0.52
1:A:150:LEU:HG	1:A:525:SER:HB2	1.92	0.52
1:A:99:ASP:CG	1:A:216:ARG:HH21	2.14	0.51
1:A:403:HIS:CD2	1:A:549:GLN:HE22	2.27	0.51
1:A:65:SER:O	1:A:530:LYS:HA	2.10	0.51
1:A:535:PHE:CD1	1:A:535:PHE:N	2.78	0.51
1:A:144:GLU:HA	1:A:262:ALA:HA	1.93	0.51
1:A:111:LEU:HD12	1:A:112:VAL:N	2.25	0.51
1:A:80:ARG:NH1	1:A:80:ARG:HG2	2.26	0.51
1:A:464:TYR:CZ	1:A:465:PRO:HB3	2.46	0.51
1:A:345:PHE:N	1:A:345:PHE:CD1	2.77	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:86:ASN:ND2	1:A:100:ASP:HB2	2.25	0.51
1:A:52:LYS:HE2	1:A:54:LEU:HD21	1.93	0.50
1:A:276:THR:OG1	1:A:581:ARG:HD3	2.11	0.50
1:A:476:THR:O	1:A:479:LYS:HE2	2.12	0.50
1:A:101:ILE:O	1:A:102:HIS:HB3	2.11	0.50
1:A:155:GLU:CB	1:A:160:PRO:HA	2.31	0.49
1:A:411:GLU:O	1:A:432:PRO:HG2	2.12	0.49
1:A:307:GLY:O	1:A:308:VAL:CG2	2.60	0.49
1:A:122:ASN:OD1	1:A:122:ASN:C	2.51	0.49
1:A:472:LYS:O	1:A:483:HIS:HE1	1.96	0.49
1:A:317:THR:CG2	1:A:329:THR:HG22	2.43	0.49
1:A:68:LEU:HD12	1:A:68:LEU:C	2.33	0.48
1:A:366:THR:HA	1:A:370:GLN:CG	2.43	0.48
1:A:533:LEU:HG	1:A:535:PHE:CE1	2.48	0.48
1:A:232:ILE:HD11	1:A:234:HIS:CE1	2.48	0.48
1:A:217:THR:HG22	1:A:218:LEU:N	2.28	0.48
1:A:472:LYS:HA	1:A:494:CYS:SG	2.54	0.47
1:A:177:LEU:HD22	1:A:263:THR:HG22	1.96	0.47
1:A:564:SER:C	1:A:566:ILE:H	2.16	0.47
1:A:557:ASN:HD22	1:A:557:ASN:N	2.12	0.47
1:A:378:TYR:O	1:A:397:ARG:HA	2.15	0.47
1:A:53:PHE:O	1:A:54:LEU:HD23	2.15	0.47
1:A:462:PRO:HD2	1:A:576:SER:OG	2.15	0.47
1:A:367:ASP:C	1:A:369:ASN:H	2.19	0.46
1:A:267:PHE:CD1	1:A:267:PHE:N	2.83	0.46
1:A:424:VAL:HG21	1:A:429:VAL:HB	1.97	0.46
1:A:201:LYS:HG3	1:A:202:PRO:O	2.15	0.46
1:A:424:VAL:CG2	1:A:429:VAL:HB	2.46	0.46
1:A:186:THR:O	1:A:186:THR:OG1	2.29	0.46
1:A:66:SER:HA	1:A:529:TRP:O	2.15	0.46
1:A:214:TRP:O	1:A:350:GLN:HG2	2.15	0.46
1:A:189:ALA:HB3	1:A:468:GLN:HG3	1.97	0.46
1:A:486:ALA:HA	1:A:487:PRO:HD3	1.81	0.46
1:A:66:SER:O	1:A:67:ARG:NH1	2.49	0.46
1:A:149:VAL:C	1:A:150:LEU:HD12	2.37	0.45
1:A:425:THR:HG22	1:A:426:ASN:N	2.31	0.45
1:A:46:ASN:C	1:A:46:ASN:OD1	2.54	0.45
1:A:266:PHE:CD1	1:A:495:PRO:HG3	2.51	0.45
1:A:236:THR:HG22	1:A:237:ASP:N	2.32	0.45
1:A:218:LEU:HD12	1:A:219:ILE:N	2.32	0.45
1:A:136:LEU:C	1:A:137:HIS:HD2	2.19	0.45
1:A:443:ASN:OD1	1:A:445:THR:N	2.50	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:455:THR:HG22	1:A:457:LEU:CD2	2.47	0.45
1:A:105:ILE:HA	1:A:105:ILE:HD13	1.76	0.45
1:A:557:ASN:ND2	1:A:557:ASN:N	2.64	0.44
1:A:322:THR:CG2	1:A:420:PHE:CD2	2.91	0.44
1:A:79:TYR:CD2	1:A:107:THR:HG22	2.52	0.44
1:A:49:THR:CG2	1:A:50:GLU:N	2.80	0.44
1:A:295:PRO:HD3	1:A:304:GLY:HA2	2.00	0.44
1:A:177:LEU:C	1:A:177:LEU:HD12	2.37	0.44
1:A:365:GLN:O	1:A:370:GLN:HG3	2.18	0.44
1:A:548:ILE:CD1	1:A:579:ALA:HB2	2.47	0.44
1:A:398:PHE:C	1:A:398:PHE:CD1	2.90	0.44
1:A:144:GLU:HB3	1:A:262:ALA:CB	2.47	0.44
1:A:583:LEU:C	1:A:583:LEU:HD23	2.38	0.44
1:A:90:THR:CG2	1:A:99:ASP:HA	2.48	0.44
1:A:127:GLN:NE2	1:A:552:SER:HA	2.33	0.44
1:A:153:VAL:HG22	1:A:165:TYR:CD1	2.53	0.44
1:A:339:SER:H	1:A:450:THR:HG1	1.62	0.43
1:A:345:PHE:HD1	1:A:345:PHE:N	2.15	0.43
1:A:86:ASN:O	1:A:87:MET:C	2.55	0.43
1:A:398:PHE:HE2	1:A:466:ASN:ND2	2.16	0.43
1:A:417:ASN:OD1	1:A:419:ASN:ND2	2.50	0.43
1:A:250:VAL:HA	1:A:251:PRO:HD3	1.88	0.43
1:A:138:LEU:HA	1:A:138:LEU:HD12	1.89	0.43
1:A:218:LEU:HD12	1:A:218:LEU:C	2.38	0.43
1:A:80:ARG:CG	1:A:80:ARG:HH11	2.32	0.43
1:A:93:ASN:HD22	1:A:225:THR:HB	1.84	0.42
1:A:564:SER:C	1:A:566:ILE:N	2.72	0.42
1:A:69:VAL:CG1	1:A:205:PRO:HD3	2.48	0.42
1:A:494:CYS:O	1:A:495:PRO:C	2.55	0.42
1:A:435:PRO:HB3	1:A:439:LYS:O	2.19	0.42
1:A:107:THR:HG21	1:A:208:TRP:CE3	2.54	0.42
1:A:377:ARG:HH11	1:A:377:ARG:HG3	1.83	0.42
1:A:221:SER:HB2	1:A:225:THR:CG2	2.45	0.42
1:A:400:TYR:CD2	1:A:463:VAL:HG13	2.55	0.42
1:A:291:LEU:HA	1:A:306:ILE:HA	2.01	0.42
1:A:321:ASN:H	1:A:321:ASN:HD22	1.68	0.42
1:A:217:THR:CG2	1:A:218:LEU:N	2.83	0.42
1:A:339:SER:HB2	1:A:450:THR:OG1	2.19	0.42
1:A:439:LYS:HA	1:A:439:LYS:HD3	1.74	0.41
1:A:191:ARG:O	1:A:192:SER:C	2.57	0.41
1:A:564:SER:O	1:A:566:ILE:N	2.53	0.41
1:A:459:ASN:OD1	1:A:460:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:389:THR:HG23	1:A:568:GLY:HA2	2.02	0.41
1:A:274:ARG:O	1:A:275:LEU:HD23	2.21	0.41
1:A:424:VAL:O	1:A:424:VAL:HG13	2.20	0.41
1:A:391:THR:C	1:A:392:GLY:O	2.58	0.41
1:A:464:TYR:CD2	1:A:465:PRO:HB3	2.55	0.41
1:A:459:ASN:OD1	1:A:460:VAL:N	2.54	0.41
1:A:569:MET:HE3	1:A:570:LYS:H	1.85	0.41
1:A:90:THR:HG21	1:A:99:ASP:HA	2.02	0.41
1:A:87:MET:HG3	1:A:231:ASN:HD22	1.85	0.41
1:A:471:ASP:OD2	1:A:483:HIS:ND1	2.51	0.41
1:A:377:ARG:NH1	1:A:377:ARG:HG3	2.36	0.41
1:A:517:ASN:HD22	1:A:517:ASN:HA	1.59	0.41
1:A:410:PRO:HG2	1:A:411:GLU:OE1	2.21	0.41
1:A:80:ARG:HG2	1:A:80:ARG:HH11	1.85	0.40
1:A:389:THR:HG23	1:A:568:GLY:CA	2.51	0.40
1:A:382:ARG:NH2	1:A:392:GLY:O	2.54	0.40
1:A:144:GLU:CB	1:A:262:ALA:HA	2.51	0.40
1:A:382:ARG:HG3	1:A:382:ARG:NH1	2.37	0.40
1:A:140:SER:O	1:A:141:PHE:HB2	2.21	0.40
1:A:193:GLU:OE1	1:A:206:THR:HG21	2.21	0.40
1:A:483:HIS:HB3	1:A:485:ASN:OD1	2.22	0.40
1:A:138:LEU:HG	1:A:268:PHE:CD2	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	542/584 (93%)	455 (84%)	70 (13%)	17 (3%)	<b>7</b> 53

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	ASN

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Mol	Chain	Res	Type
1	A	330	ILE
1	A	349	THR
1	A	361	ARG
1	A	558	GLN
1	A	88	ASP
1	A	178	ASP
1	A	141	PHE
1	A	181	ASN
1	A	57	GLY
1	A	271	LYS
1	A	321	ASN
1	A	492	ASN
1	A	513	ASP
1	A	453	PRO
1	A	418	ILE
1	A	160	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	473/495 (96%)	436 (92%)	37 (8%)	18 63

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

Mol	Chain	Res	Type
1	A	68	LEU
1	A	80	ARG
1	A	87	MET
1	A	95	ASN
1	A	96	MET
1	A	133	MET
1	A	136	LEU
1	A	154	SER
1	A	166	ASN
1	A	178	ASP
1	A	186	THR
1	A	201	LYS

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Mol	Chain	Res	Type
1	A	209	ARG
1	A	216	ARG
1	A	218	LEU
1	A	260	GLU
1	A	261	PHE
1	A	281	THR
1	A	339	SER
1	A	344	SER
1	A	345	PHE
1	A	350	GLN
1	A	354	LYS
1	A	384	HIS
1	A	390	THR
1	A	398	PHE
1	A	422	LEU
1	A	444	TYR
1	A	446	ASN
1	A	457	LEU
1	A	465	PRO
1	A	490	CYS
1	A	497	GLN
1	A	517	ASN
1	A	535	PHE
1	A	557	ASN
1	A	572	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	127	GLN
1	A	181	ASN
1	A	242	GLN
1	A	309	GLN
1	A	321	ASN
1	A	365	GLN
1	A	375	ASN
1	A	383	GLN
1	A	386	GLN
1	A	416	GLN
1	A	466	ASN
1	A	491	GLN

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Mol	Chain	Res	Type
1	A	492	ASN
1	A	517	ASN
1	A	549	GLN
1	A	557	ASN
1	A	560	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	544/584 (93%)	1.09	25 (4%) 31 14	9, 32, 71, 100	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	372	ALA	2.8
1	A	228	THR	2.5
1	A	495	PRO	2.5
1	A	365	GLN	2.4
1	A	494	CYS	2.4
1	A	338	TYR	2.4
1	A	96	MET	2.4
1	A	375	ASN	2.3
1	A	359	ALA	2.3
1	A	362	GLY	2.2
1	A	91	ALA	2.2
1	A	90	THR	2.2
1	A	230	THR	2.2
1	A	203	THR	2.1
1	A	368	GLU	2.1
1	A	425	THR	2.1
1	A	227	GLY	2.1
1	A	379	ALA	2.1
1	A	225	THR	2.1
1	A	401	ILE	2.1
1	A	422	LEU	2.0
1	A	497	GLN	2.0
1	A	136	LEU	2.0
1	A	95	ASN	2.0
1	A	107	THR	2.0



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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CA	A	586	1/1	0.13	-17.05	40,40,40,40	0
2	CA	A	585	1/1	0.23	-	40,40,40,40	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.