



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:29 AM GMT

PDB ID : 1C8D  
Title : CANINE PANLEUKOPENIA VIRUS EMPTY CAPSID STRUCTURE  
Authors : Rossmann, M.G.; Simpson, A.A.  
Deposited on : 2000-05-05  
Resolution : 3.00 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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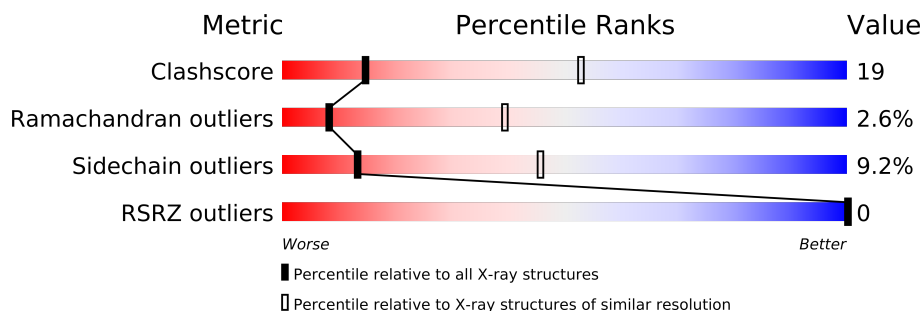
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.00 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	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, blue);"></div> </div>

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	CA	A	585	-	X

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4353 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
1	A	548	Total	C	N	O	S	0	0	0
			4352	2765	742	829	16			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	267.56Å 268.45Å 274.33Å 61.95° 62.62° 60.19°	Depositor
Resolution (Å)	9.00 – 3.00 39.84 – 3.00	Depositor EDS
% Data completeness (in resolution range)	31.3 (9.00-3.00) 31.4 (39.84-3.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	9.56 (at 3.01Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, $R_{free}$	0.214 , (Not available) 0.218 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	30.2	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 73.3	EDS
Estimated twinning fraction	0.013 for -h+k,-h,-h+l 0.013 for -k,h-k,-k+l 0.029 for h,h-k,h-l 0.035 for -h+k,k,k-l 0.017 for -k,-h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 351740 reflections	Xtriage
$F_o, F_c$ correlation	0.12	EDS
Total number of atoms	4353	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.88% 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	0.40	0/4482	0.71	3/6133 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	366	THR	N-CA-C	-5.65	95.75	111.00
1	A	583	LEU	CA-CB-CG	5.45	127.84	115.30
1	A	367	ASP	N-CA-C	-5.16	97.06	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	4352	0	4144	163	0
2	A	1	0	0	0	0
All	All	4353	0	4144	163	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 19.

All (163) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:485:ASN:H	1:A:485:ASN:HD22	1.09	1.00
1:A:276:THR:HG22	1:A:581:ARG:HH11	1.30	0.97
1:A:133:MET:HG2	1:A:537:ALA:HB1	1.47	0.96
1:A:193:GLU:HB3	1:A:206:THR:HG21	1.46	0.95
1:A:554:ASN:H	1:A:557:ASN:HD21	1.14	0.94
1:A:157:ALA:HA	1:A:161:PRO:HB2	1.51	0.93
1:A:159:GLN:HB2	1:A:160:PRO:CD	2.00	0.92
1:A:557:ASN:HD22	1:A:558:GLN:N	1.69	0.89
1:A:159:GLN:HB2	1:A:160:PRO:HD2	1.57	0.86
1:A:459:ASN:ND2	1:A:460:VAL:H	1.71	0.86
1:A:160:PRO:HG2	1:A:161:PRO:C	1.95	0.85
1:A:414:TRP:HE1	1:A:416:GLN:HE21	1.26	0.80
1:A:326:THR:HG22	1:A:328:ALA:H	1.47	0.80
1:A:485:ASN:ND2	1:A:485:ASN:H	1.81	0.78
1:A:133:MET:HG2	1:A:537:ALA:CB	2.13	0.77
1:A:263:THR:HG22	1:A:264:GLY:O	1.84	0.77
1:A:245:THR:HG22	1:A:248:ASN:H	1.50	0.77
1:A:381:GLY:HA2	1:A:386:GLN:HB3	1.65	0.76
1:A:160:PRO:HG3	1:A:162:THR:HG23	1.66	0.75
1:A:85:ASN:C	1:A:85:ASN:HD22	1.87	0.75
1:A:101:ILE:HD11	1:A:233:TYR:HD1	1.50	0.75
1:A:485:ASN:N	1:A:485:ASN:HD22	1.85	0.75
1:A:96:MET:H	1:A:96:MET:HE2	1.55	0.72
1:A:122:ASN:ND2	1:A:125:ASP:H	1.88	0.71
1:A:554:ASN:H	1:A:557:ASN:ND2	1.86	0.71
1:A:361:ARG:HD2	1:A:361:ARG:O	1.91	0.69
1:A:85:ASN:HD21	1:A:87:MET:HB2	1.56	0.69
1:A:554:ASN:N	1:A:557:ASN:HD21	1.90	0.69
1:A:431:LEU:C	1:A:433:THR:H	1.96	0.69
1:A:157:ALA:HA	1:A:161:PRO:CB	2.24	0.68
1:A:73:MET:CE	1:A:522:VAL:HA	2.24	0.68
1:A:213:GLN:HG3	1:A:240:ASP:CB	2.24	0.68
1:A:276:THR:HG22	1:A:581:ARG:NH1	2.07	0.67
1:A:183:MET:HG2	1:A:208:TRP:CH2	2.30	0.67
1:A:52:LYS:HB3	1:A:60:TYR:HB3	1.76	0.67
1:A:92:VAL:HB	1:A:95:ASN:HD22	1.59	0.67
1:A:42:THR:H	1:A:147:ASN:HD21	1.43	0.66
1:A:317:THR:CG2	1:A:319:MET:H	2.09	0.66
1:A:160:PRO:HG2	1:A:162:THR:N	2.10	0.66
1:A:424:VAL:HG22	1:A:429:VAL:HG22	1.77	0.66
1:A:158:THR:O	1:A:161:PRO:HA	1.96	0.65
1:A:381:GLY:O	1:A:383:GLN:N	2.30	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:390:THR:HG22	1:A:391:THR:N	2.13	0.64
1:A:158:THR:H	1:A:161:PRO:CB	2.11	0.63
1:A:122:ASN:C	1:A:122:ASN:HD22	2.02	0.63
1:A:282:ASN:HD21	1:A:335:GLU:HA	1.63	0.63
1:A:317:THR:HG23	1:A:319:MET:H	1.62	0.63
1:A:42:THR:H	1:A:147:ASN:ND2	1.96	0.63
1:A:339:SER:O	1:A:449:ASN:HA	1.99	0.63
1:A:282:ASN:ND2	1:A:336:VAL:H	1.97	0.63
1:A:420:PHE:O	1:A:421:ASN:HB2	1.98	0.63
1:A:158:THR:O	1:A:160:PRO:HD2	1.98	0.62
1:A:159:GLN:HA	1:A:159:GLN:HE21	1.64	0.62
1:A:47:ASN:HD21	1:A:67:ARG:HH11	1.46	0.62
1:A:269:ASP:O	1:A:491:GLN:HG3	1.99	0.61
1:A:159:GLN:CB	1:A:160:PRO:CD	2.77	0.61
1:A:154:SER:HB3	1:A:164:VAL:HB	1.83	0.60
1:A:578:LEU:O	1:A:579:ALA:CB	2.48	0.60
1:A:425:THR:HG22	1:A:427:ASP:H	1.66	0.60
1:A:213:GLN:HG3	1:A:240:ASP:HB3	1.82	0.60
1:A:557:ASN:HD22	1:A:557:ASN:C	2.04	0.60
1:A:276:THR:HG21	1:A:581:ARG:HD3	1.83	0.59
1:A:193:GLU:HB3	1:A:206:THR:CG2	2.26	0.59
1:A:282:ASN:HD21	1:A:336:VAL:H	1.50	0.58
1:A:297:SER:HB2	1:A:302:ASN:ND2	2.18	0.58
1:A:322:THR:HG21	1:A:420:PHE:CD1	2.38	0.58
1:A:459:ASN:ND2	1:A:460:VAL:N	2.48	0.58
1:A:96:MET:N	1:A:96:MET:HE2	2.18	0.58
1:A:362:GLY:H	1:A:407:GLY:H	1.49	0.58
1:A:215:ASP:HB3	1:A:234:HIS:HB2	1.87	0.57
1:A:424:VAL:CG2	1:A:429:VAL:HG22	2.34	0.57
1:A:158:THR:N	1:A:161:PRO:HB3	2.21	0.56
1:A:216:ARG:C	1:A:216:ARG:HD3	2.26	0.56
1:A:85:ASN:C	1:A:85:ASN:ND2	2.58	0.55
1:A:324:TYR:O	1:A:329:THR:HG21	2.07	0.55
1:A:382:ARG:HG2	1:A:382:ARG:HH11	1.71	0.55
1:A:133:MET:CE	1:A:539:LEU:HD23	2.36	0.55
1:A:326:THR:HG22	1:A:327:GLU:N	2.20	0.55
1:A:73:MET:HE2	1:A:522:VAL:HA	1.88	0.55
1:A:213:GLN:HG3	1:A:240:ASP:HB2	1.87	0.54
1:A:321:ASN:H	1:A:321:ASN:HD22	1.55	0.54
1:A:276:THR:CG2	1:A:581:ARG:HH11	2.10	0.54
1:A:367:ASP:C	1:A:368:GLU:HG3	2.28	0.54
1:A:216:ARG:CZ	1:A:218:LEU:HB2	2.38	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:368:GLU:CD	1:A:369:ASN:H	2.12	0.52
1:A:73:MET:HE1	1:A:522:VAL:HA	1.90	0.52
1:A:266:PHE:CD1	1:A:495:PRO:HG3	2.45	0.51
1:A:85:ASN:ND2	1:A:87:MET:HB2	2.25	0.51
1:A:321:ASN:HD22	1:A:321:ASN:N	2.08	0.51
1:A:183:MET:CG	1:A:208:TRP:CH2	2.93	0.50
1:A:116:ALA:HA	1:A:467:GLY:O	2.12	0.50
1:A:122:ASN:HB2	1:A:123:PRO:HD2	1.94	0.50
1:A:160:PRO:CG	1:A:162:THR:HG23	2.37	0.50
1:A:276:THR:HG21	1:A:581:ARG:HB3	1.92	0.50
1:A:483:HIS:HB3	1:A:485:ASN:ND2	2.26	0.49
1:A:276:THR:CG2	1:A:581:ARG:HB3	2.42	0.49
1:A:101:ILE:CD1	1:A:233:TYR:HD1	2.23	0.49
1:A:340:ALA:HB3	1:A:357:ILE:HD12	1.94	0.49
1:A:336:VAL:O	1:A:408:ARG:NH2	2.45	0.49
1:A:562:VAL:HG13	1:A:563:PRO:HD2	1.94	0.49
1:A:390:THR:CG2	1:A:391:THR:N	2.76	0.49
1:A:182:THR:HG22	1:A:183:MET:HE3	1.95	0.49
1:A:431:LEU:C	1:A:433:THR:N	2.65	0.49
1:A:183:MET:CG	1:A:208:TRP:HH2	2.27	0.48
1:A:158:THR:N	1:A:161:PRO:CB	2.74	0.48
1:A:194:THR:HG23	1:A:195:LEU:O	2.14	0.48
1:A:562:VAL:HG13	1:A:563:PRO:CD	2.44	0.47
1:A:326:THR:CG2	1:A:327:GLU:N	2.77	0.47
1:A:368:GLU:O	1:A:369:ASN:CB	2.62	0.47
1:A:219:ILE:HD12	1:A:230:THR:HB	1.97	0.47
1:A:459:ASN:HD22	1:A:460:VAL:H	1.59	0.47
1:A:245:THR:HG21	1:A:248:ASN:OD1	2.15	0.47
1:A:321:ASN:H	1:A:321:ASN:ND2	2.13	0.47
1:A:217:THR:OG1	1:A:234:HIS:HE1	1.97	0.47
1:A:47:ASN:ND2	1:A:66:SER:H	2.12	0.47
1:A:212:PHE:O	1:A:214:TRP:HE3	1.97	0.46
1:A:43:GLY:HA3	1:A:146:PHE:CD1	2.51	0.46
1:A:92:VAL:HB	1:A:95:ASN:ND2	2.27	0.45
1:A:193:GLU:OE2	1:A:206:THR:HG21	2.17	0.45
1:A:245:THR:HG23	1:A:247:GLU:OE1	2.16	0.45
1:A:122:ASN:HD22	1:A:125:ASP:H	1.64	0.45
1:A:70:HIS:HD2	1:A:526:ASP:OD2	1.99	0.45
1:A:122:ASN:C	1:A:122:ASN:ND2	2.70	0.45
1:A:77:GLU:OE1	1:A:520:ARG:NH1	2.49	0.45
1:A:183:MET:HG3	1:A:208:TRP:HH2	1.82	0.44
1:A:378:TYR:O	1:A:397:ARG:HA	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:113:ASP:OD2	1:A:113:ASP:C	2.56	0.44
1:A:483:HIS:HB3	1:A:485:ASN:HD21	1.81	0.44
1:A:54:LEU:N	1:A:54:LEU:HD13	2.33	0.44
1:A:70:HIS:CD2	1:A:526:ASP:OD2	2.71	0.44
1:A:420:PHE:HB3	1:A:421:ASN:H	1.73	0.44
1:A:216:ARG:NH2	1:A:231:ASN:OD1	2.51	0.44
1:A:229:PRO:O	1:A:230:THR:CB	2.66	0.43
1:A:341:PRO:HB3	1:A:447:ILE:HA	1.99	0.43
1:A:96:MET:HG2	1:A:220:PRO:HA	2.00	0.43
1:A:536:LYS:HE3	1:A:536:LYS:HB2	1.74	0.43
1:A:160:PRO:HG2	1:A:161:PRO:CA	2.47	0.43
1:A:362:GLY:H	1:A:407:GLY:N	2.14	0.43
1:A:51:PHE:CZ	1:A:128:LEU:HD23	2.54	0.43
1:A:155:GLU:O	1:A:157:ALA:N	2.45	0.43
1:A:370:GLN:NE2	1:A:401:ILE:HD11	2.34	0.42
1:A:38:VAL:HG21	1:A:169:LEU:HD13	2.01	0.42
1:A:377:ARG:HH11	1:A:377:ARG:HG3	1.83	0.42
1:A:322:THR:HG21	1:A:420:PHE:HD1	1.84	0.42
1:A:578:LEU:O	1:A:579:ALA:HB3	2.20	0.42
1:A:411:GLU:CD	1:A:411:GLU:H	2.23	0.42
1:A:548:ILE:HA	1:A:548:ILE:HD12	1.69	0.42
1:A:266:PHE:CE1	1:A:495:PRO:HG3	2.55	0.42
1:A:183:MET:CE	1:A:244:TYR:HB3	2.50	0.42
1:A:185:PHE:CD2	1:A:187:PRO:HD3	2.56	0.41
1:A:141:PHE:CZ	1:A:143:GLN:HG2	2.56	0.41
1:A:237:ASP:HA	1:A:238:PRO:HD3	1.93	0.41
1:A:294:LEU:HA	1:A:295:PRO:HD3	1.94	0.41
1:A:159:GLN:HB2	1:A:160:PRO:HD3	1.95	0.41
1:A:367:ASP:O	1:A:368:GLU:HG3	2.20	0.41
1:A:566:ILE:CG2	1:A:566:ILE:O	2.69	0.41
1:A:473:GLU:HG3	1:A:474:PHE:N	2.36	0.41
1:A:557:ASN:HD22	1:A:558:GLN:H	1.59	0.40
1:A:158:THR:O	1:A:160:PRO:CD	2.68	0.40
1:A:382:ARG:HG2	1:A:382:ARG:NH1	2.34	0.40
1:A:159:GLN:HA	1:A:159:GLN:NE2	2.33	0.40
1:A:293:SER:HB3	1:A:305:ASP:HB3	2.03	0.40
1:A:224:GLY:O	1:A:225:THR:C	2.60	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	546/584 (94%)	500 (92%)	32 (6%)	14 (3%)	8 39

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	GLN
1	A	230	THR
1	A	366	THR
1	A	382	ARG
1	A	518	MET
1	A	579	ALA
1	A	368	GLU
1	A	369	ASN
1	A	362	GLY
1	A	157	ALA
1	A	492	ASN
1	A	156	SER
1	A	349	THR
1	A	558	GLN

### 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	477/496 (96%)	433 (91%)	44 (9%)	13 46

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LEU
1	A	67	ARG
1	A	85	ASN
1	A	87	MET
1	A	96	MET
1	A	101	ILE
1	A	111	LEU
1	A	122	ASN
1	A	133	MET
1	A	152	THR
1	A	159	GLN
1	A	162	THR
1	A	177	LEU
1	A	183	MET
1	A	195	LEU
1	A	209	ARG
1	A	215	ASP
1	A	216	ARG
1	A	263	THR
1	A	276	THR
1	A	317	THR
1	A	321	ASN
1	A	350	GLN
1	A	354	LYS
1	A	365	GLN
1	A	368	GLU
1	A	382	ARG
1	A	388	THR
1	A	391	THR
1	A	393	GLU
1	A	420	PHE
1	A	429	VAL
1	A	431	LEU
1	A	433	THR
1	A	465	PRO
1	A	485	ASN
1	A	494	CYS
1	A	509	GLN
1	A	513	ASP
1	A	518	MET
1	A	548	ILE
1	A	557	ASN
1	A	578	LEU

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Mol	Chain	Res	Type
1	A	583	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	70	HIS
1	A	85	ASN
1	A	95	ASN
1	A	122	ASN
1	A	147	ASN
1	A	159	GLN
1	A	234	HIS
1	A	242	GLN
1	A	282	ASN
1	A	292	ASN
1	A	310	GLN
1	A	321	ASN
1	A	370	GLN
1	A	383	GLN
1	A	384	HIS
1	A	403	HIS
1	A	416	GLN
1	A	443	ASN
1	A	459	ASN
1	A	468	GLN
1	A	485	ASN
1	A	492	ASN
1	A	546	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 1 ligands modelled in this entry, 1 is 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	548/584 (93%)	-0.40	0 100 100	3, 14, 44, 78	0

There are no RSRZ outliers to report.

### 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	585	1/1	0.21	4.77	30,30,30,30	1

### 6.5 Other polymers ⓘ

There are no such residues in this entry.