Full wwPDB X-ray Structure Validation Report (i)

Apr 29, 2025 – 01:40 PM EDT

PDB ID	:	1C8D / pdb_00001c8d
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 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

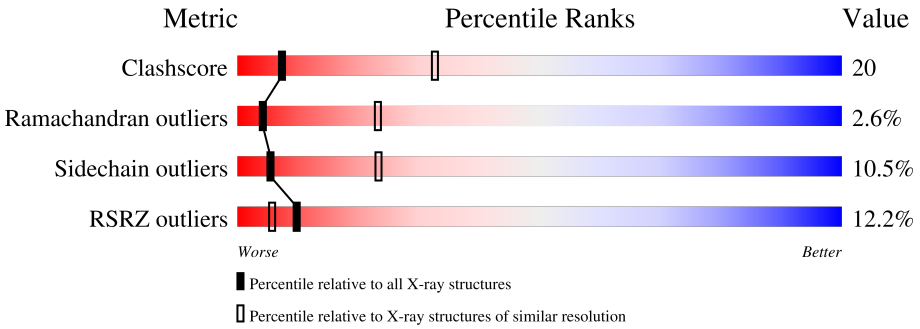
MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 3.00 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	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (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 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	584	11% 61% 24% 8% • 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4353 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 CANINE PARVOVIRUS CAPSID.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	548	4352	2765	742	829	16	0	0	0

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	A	1	1	1	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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

- Molecule 1: CANINE PARVOVIRUS CAPSID

Chain A:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	267.56Å 268.45Å 274.33Å 61.95° 62.62° 60.19°	Depositor
Resolution (Å)	9.00 – 3.00 9.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	31.3 (9.00-3.00) 30.5 (9.00-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	9.56 (at 3.01Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.214 , (Not available) 0.214 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	30.2	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 91.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
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
F_o,F_c correlation	0.13	EDS
Total number of atoms	4353	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.50	0/4482	1.07	26/6133 (0.4%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	444	TYR	N-CA-C	-11.74	99.08	113.41
1	A	228	THR	CA-C-N	9.07	131.18	119.84
1	A	228	THR	C-N-CA	9.07	131.18	119.84
1	A	367	ASP	N-CA-C	-8.09	97.06	109.85
1	A	366	THR	N-CA-C	-7.08	95.71	110.80
1	A	576	SER	N-CA-C	6.62	121.49	113.41
1	A	342	TYR	N-CA-C	6.62	119.73	109.07
1	A	583	LEU	N-CA-C	-6.54	103.98	112.68
1	A	381	GLY	N-CA-C	6.49	120.58	110.91
1	A	232	ILE	N-CA-C	6.29	117.53	108.48
1	A	578	LEU	N-CA-C	-5.91	100.36	109.76
1	A	160	PRO	N-CA-C	5.86	117.85	110.70
1	A	416	GLN	N-CA-C	5.78	118.19	109.23
1	A	120	TRP	N-CA-C	5.72	120.39	113.41
1	A	397	ARG	N-CA-C	5.63	116.82	108.60
1	A	468	GLN	N-CA-C	-5.47	102.38	110.48
1	A	159	GLN	CA-C-N	-5.44	114.77	120.38
1	A	159	GLN	C-N-CA	-5.44	114.77	120.38
1	A	350	GLN	N-CA-C	5.44	119.48	112.41
1	A	506	LEU	N-CA-C	5.31	117.98	110.50
1	A	304	GLY	N-CA-C	-5.26	104.27	112.58
1	A	303	PHE	N-CA-C	5.23	117.61	110.55
1	A	130	VAL	N-CA-C	5.20	116.55	110.62
1	A	82	VAL	N-CA-C	5.16	115.91	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	237	ASP	CA-C-N	5.10	125.14	119.32
1	A	237	ASP	C-N-CA	5.10	125.14	119.32

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	4352	0	4144	172	0
2	A	1	0	0	0	0
All	All	4353	0	4144	172	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 20.

All (172) 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:485:ASN:H	1:A:485:ASN:HD22	1.09	1.00
1:A:193:GLU:HB3	1:A:206:THR:HG21	1.45	0.97
1:A:133:MET:HG2	1:A:537:ALA:HB1	1.47	0.96
1:A:276:THR:HG22	1:A:581:ARG:HH11	1.30	0.94
1:A:159:GLN:HB2	1:A:160:PRO:CD	2.00	0.92
1:A:157:ALA:HA	1:A:161:PRO:HB2	1.50	0.91
1:A:160:PRO:HG2	1:A:161:PRO:C	1.95	0.91
1:A:557:ASN:HD22	1:A:558:GLN:N	1.69	0.89
1:A:459:ASN:ND2	1:A:460:VAL:H	1.71	0.89
1:A:554:ASN:H	1:A:557:ASN:HD21	1.14	0.88
1:A:159:GLN:HB2	1:A:160:PRO:HD2	1.57	0.86
1:A:414:TRP:HE1	1:A:416:GLN:HE21	1.26	0.82
1:A:85:ASN:C	1:A:85:ASN:HD22	1.87	0.81
1:A:326:THR:HG22	1:A:328:ALA:H	1.47	0.80
1:A:381:GLY:HA2	1:A:386:GLN:HB3	1.65	0.79
1:A:133:MET:HG2	1:A:537:ALA:CB	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:PRO:HG3	1:A:162:THR:HG23	1.66	0.77
1:A:73:MET:HE1	1:A:522:VAL:HA	1.66	0.77
1:A:101:ILE:HD11	1:A:233:TYR:HD1	1.50	0.76
1:A:263:THR:HG22	1:A:264:GLY:O	1.84	0.75
1:A:485:ASN:HD22	1:A:485:ASN:N	1.85	0.74
1:A:174:MET:HE2	1:A:252:VAL:HG11	1.70	0.73
1:A:431:LEU:C	1:A:433:THR:H	1.96	0.73
1:A:245:THR:HG22	1:A:248:ASN:H	1.50	0.73
1:A:485:ASN:H	1:A:485:ASN:ND2	1.81	0.72
1:A:183:MET:HE2	1:A:244:TYR:HB3	1.72	0.71
1:A:122:ASN:ND2	1:A:125:ASP:H	1.88	0.71
1:A:85:ASN:HD21	1:A:87:MET:HB2	1.56	0.70
1:A:361:ARG:O	1:A:361:ARG:HD2	1.92	0.70
1:A:554:ASN:H	1:A:557:ASN:ND2	1.86	0.69
1:A:554:ASN:N	1:A:557:ASN:HD21	1.90	0.68
1:A:122:ASN:C	1:A:122:ASN:HD22	2.02	0.68
1:A:52:LYS:HB3	1:A:60:TYR:HB3	1.76	0.68
1:A:157:ALA:HA	1:A:161:PRO:CB	2.24	0.67
1:A:213:GLN:HG3	1:A:240:ASP:CB	2.24	0.67
1:A:160:PRO:HG2	1:A:162:THR:N	2.10	0.67
1:A:424:VAL:HG22	1:A:429:VAL:HG22	1.77	0.66
1:A:92:VAL:HB	1:A:95:ASN:HD22	1.59	0.66
1:A:73:MET:CE	1:A:522:VAL:HA	2.24	0.66
1:A:317:THR:CG2	1:A:319:MET:H	2.09	0.66
1:A:42:THR:H	1:A:147:ASN:HD21	1.43	0.66
1:A:183:MET:HG2	1:A:208:TRP:CH2	2.30	0.66
1:A:276:THR:HG22	1:A:581:ARG:NH1	2.07	0.66
1:A:557:ASN:HD22	1:A:557:ASN:C	2.04	0.65
1:A:158:THR:O	1:A:161:PRO:HA	1.96	0.65
1:A:317:THR:HG23	1:A:319:MET:H	1.62	0.65
1:A:158:THR:O	1:A:160:PRO:HD2	1.98	0.64
1:A:158:THR:H	1:A:161:PRO:CB	2.11	0.64
1:A:390:THR:HG22	1:A:391:THR:N	2.13	0.63
1:A:381:GLY:O	1:A:383:GLN:N	2.30	0.63
1:A:282:ASN:ND2	1:A:336:VAL:H	1.97	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:193:GLU:HB3	1:A:206:THR:CG2	2.26	0.62
1:A:159:GLN:HE21	1:A:159:GLN:HA	1.64	0.62
1:A:269:ASP:O	1:A:491:GLN:HG3	1.99	0.62
1:A:47:ASN:HD21	1:A:67:ARG:HH11	1.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ASN:HD21	1:A:335:GLU:HA	1.63	0.62
1:A:420:PHE:O	1:A:421:ASN:HB2	1.98	0.61
1:A:578:LEU:O	1:A:579:ALA:CB	2.48	0.61
1:A:216:ARG:C	1:A:216:ARG:HD3	2.26	0.60
1:A:425:THR:HG22	1:A:427:ASP:H	1.66	0.60
1:A:154:SER:HB3	1:A:164:VAL:HB	1.82	0.60
1:A:213:GLN:HG3	1:A:240:ASP:HB3	1.82	0.60
1:A:362:GLY:H	1:A:407:GLY:H	1.50	0.59
1:A:276:THR:HG21	1:A:581:ARG:HD3	1.83	0.59
1:A:297:SER:HB2	1:A:302:ASN:ND2	2.18	0.59
1:A:322:THR:HG21	1:A:420:PHE:CD1	2.38	0.59
1:A:159:GLN:CB	1:A:160:PRO:CD	2.77	0.58
1:A:367:ASP:C	1:A:368:GLU:HG3	2.28	0.58
1:A:282:ASN:HD21	1:A:336:VAL:H	1.50	0.58
1:A:424:VAL:CG2	1:A:429:VAL:HG22	2.34	0.57
1:A:85:ASN:C	1:A:85:ASN:ND2	2.58	0.57
1:A:459:ASN:ND2	1:A:460:VAL:N	2.48	0.57
1:A:518:MET:HE1	1:A:520:ARG:HG2	1.86	0.57
1:A:215:ASP:HB3	1:A:234:HIS:HB2	1.87	0.57
1:A:368:GLU:CD	1:A:369:ASN:H	2.12	0.56
1:A:158:THR:N	1:A:161:PRO:HB3	2.21	0.56
1:A:213:GLN:HG3	1:A:240:ASP:HB2	1.87	0.56
1:A:326:THR:HG22	1:A:327:GLU:N	2.20	0.56
1:A:133:MET:CE	1:A:539:LEU:HD23	2.36	0.56
1:A:382:ARG:HH11	1:A:382:ARG:HG2	1.71	0.55
1:A:324:TYR:O	1:A:329:THR:HG21	2.07	0.55
1:A:321:ASN:H	1:A:321:ASN:HD22	1.55	0.54
1:A:216:ARG:CZ	1:A:218:LEU:HB2	2.38	0.53
1:A:276:THR:CG2	1:A:581:ARG:HH11	2.10	0.53
1:A:96:MET:HE2	1:A:96:MET:H	1.73	0.52
1:A:276:THR:HG21	1:A:581:ARG:HB3	1.93	0.51
1:A:266:PHE:CD1	1:A:495:PRO:HG3	2.45	0.51
1:A:483:HIS:HB3	1:A:485:ASN:ND2	2.26	0.51
1:A:183:MET:CG	1:A:208:TRP:CH2	2.93	0.51
1:A:101:ILE:CD1	1:A:233:TYR:HD1	2.23	0.51
1:A:321:ASN:HD22	1:A:321:ASN:N	2.09	0.51
1:A:160:PRO:CG	1:A:162:THR:HG23	2.37	0.50
1:A:431:LEU:C	1:A:433:THR:N	2.65	0.50
1:A:116:ALA:HA	1:A:467:GLY:O	2.12	0.50
1:A:92:VAL:HB	1:A:95:ASN:ND2	2.27	0.50
1:A:158:THR:N	1:A:161:PRO:CB	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ASN:ND2	1:A:87:MET:HB2	2.25	0.49
1:A:122:ASN:HB2	1:A:123:PRO:HD2	1.94	0.49
1:A:340:ALA:HB3	1:A:357:ILE:HD12	1.94	0.49
1:A:459:ASN:HD22	1:A:460:VAL:H	1.59	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	0.48
1:A:276:THR:CG2	1:A:581:ARG:HB3	2.42	0.48
1:A:336:VAL:O	1:A:408:ARG:NH2	2.45	0.48
1:A:183:MET:HE2	1:A:244:TYR:CB	2.43	0.48
1:A:326:THR:CG2	1:A:327:GLU:N	2.77	0.48
1:A:183:MET:CG	1:A:208:TRP:HH2	2.27	0.48
1:A:562:VAL:HG13	1:A:563:PRO:CD	2.44	0.48
1:A:212:PHE:O	1:A:214:TRP:HE3	1.97	0.48
1:A:217:THR:OG1	1:A:234:HIS:HE1	1.97	0.48
1:A:113:ASP:C	1:A:113:ASP:OD2	2.56	0.48
1:A:155:GLU:O	1:A:157:ALA:N	2.45	0.48
1:A:368:GLU:O	1:A:369:ASN:CB	2.62	0.47
1:A:548:ILE:HD12	1:A:548:ILE:HA	1.69	0.47
1:A:194:THR:HG23	1:A:195:LEU:O	2.14	0.47
1:A:47:ASN:ND2	1:A:66:SER:H	2.12	0.47
1:A:219:ILE:HD12	1:A:230:THR:HB	1.97	0.47
1:A:321:ASN:H	1:A:321:ASN:ND2	2.13	0.47
1:A:411:GLU:H	1:A:411:GLU:CD	2.22	0.47
1:A:245:THR:HG21	1:A:248:ASN:OD1	2.15	0.46
1:A:122:ASN:ND2	1:A:122:ASN:C	2.70	0.46
1:A:94:GLY:C	1:A:96:MET:HE2	2.41	0.46
1:A:483:HIS:HB3	1:A:485:ASN:HD21	1.81	0.45
1:A:43:GLY:HA3	1:A:146:PHE:CD1	2.51	0.45
1:A:193:GLU:OE2	1:A:206:THR:HG21	2.17	0.45
1:A:70:HIS:HD2	1:A:526:ASP:OD2	2.00	0.45
1:A:183:MET:HG3	1:A:208:TRP:HH2	1.82	0.45
1:A:224:GLY:O	1:A:225:THR:C	2.60	0.45
1:A:245:THR:HG23	1:A:247:GLU:OE1	2.16	0.45
1:A:362:GLY:H	1:A:407:GLY:N	2.14	0.45
1:A:557:ASN:ND2	1:A:557:ASN:C	2.75	0.45
1:A:518:MET:HE1	1:A:520:ARG:CG	2.47	0.44
1:A:341:PRO:HB3	1:A:447:ILE:HA	1.99	0.44
1:A:77:GLU:OE1	1:A:520:ARG:NH1	2.49	0.44
1:A:54:LEU:N	1:A:54:LEU:HD13	2.33	0.44
1:A:299:GLY:C	1:A:301:THR:H	2.26	0.44
1:A:378:TYR:O	1:A:397:ARG:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ASP:C	1:A:368:GLU:CG	2.91	0.44
1:A:377:ARG:HG3	1:A:377:ARG:HH11	1.83	0.43
1:A:216:ARG:NH2	1:A:231:ASN:OD1	2.51	0.43
1:A:322:THR:HG21	1:A:420:PHE:HD1	1.84	0.43
1:A:160:PRO:HG2	1:A:161:PRO:CA	2.47	0.43
1:A:70:HIS:CD2	1:A:526:ASP:OD2	2.71	0.43
1:A:38:VAL:HG21	1:A:169:LEU:HD13	2.01	0.43
1:A:229:PRO:O	1:A:230:THR:CB	2.66	0.43
1:A:96:MET:HG2	1:A:220:PRO:HA	2.00	0.42
1:A:382:ARG:HG2	1:A:382:ARG:NH1	2.34	0.42
1:A:536:LYS:HE3	1:A:536:LYS:HB2	1.74	0.42
1:A:51:PHE:CZ	1:A:128:LEU:HD23	2.54	0.42
1:A:317:THR:HG23	1:A:319:MET:N	2.33	0.42
1:A:370:GLN:NE2	1:A:401:ILE:HD11	2.34	0.42
1:A:578:LEU:O	1:A:579:ALA:HB3	2.20	0.42
1:A:122:ASN:HD22	1:A:125:ASP:H	1.64	0.42
1:A:193:GLU:CB	1:A:206:THR:HG21	2.33	0.42
1:A:219:ILE:HA	1:A:220:PRO:HD3	1.86	0.42
1:A:367:ASP:O	1:A:368:GLU:HG3	2.20	0.41
1:A:266:PHE:CE1	1:A:495:PRO:HG3	2.55	0.41
1:A:159:GLN:HA	1:A:159:GLN:NE2	2.33	0.41
1:A:557:ASN:HD22	1:A:558:GLN:H	1.59	0.41
1:A:133:MET:HE3	1:A:539:LEU:HD23	2.02	0.41
1:A:473:GLU:HG3	1:A:474:PHE:N	2.36	0.41
1:A:379:ALA:HA	1:A:396:GLU:O	2.21	0.41
1:A:183:MET:HE2	1:A:244:TYR:CG	2.55	0.41
1:A:566:ILE:O	1:A:566:ILE:CG2	2.69	0.41
1:A:185:PHE:CD2	1:A:187:PRO:HD3	2.56	0.41
1:A:293:SER:HB3	1:A:305:ASP:HB3	2.03	0.41
1:A:141:PHE:CZ	1:A:143:GLN:HG2	2.56	0.40
1:A:545:TRP:CD1	1:A:545:TRP:C	3.00	0.40
1:A:557:ASN:O	1:A:558:GLN:C	2.64	0.40
1:A:321:ASN:N	1:A:321:ASN:ND2	2.70	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%)	4 23

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	349	THR
1	A	558	GLN
1	A	156	SER

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%)	427 (90%)	50 (10%)	5 23

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	VAL
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	162	THR
1	A	177	LEU
1	A	183	MET
1	A	195	LEU
1	A	206	THR
1	A	216	ARG
1	A	229	PRO
1	A	245	THR
1	A	263	THR
1	A	276	THR
1	A	282	ASN
1	A	317	THR
1	A	321	ASN
1	A	329	THR
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	425	THR
1	A	429	VAL
1	A	431	LEU
1	A	433	THR
1	A	440	THR
1	A	447	ILE
1	A	465	PRO
1	A	485	ASN
1	A	494	CYS

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Mol	Chain	Res	Type
1	A	509	GLN
1	A	513	ASP
1	A	518	MET
1	A	548	ILE
1	A	557	ASN
1	A	578	LEU
1	A	583	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	70	HIS
1	A	72	ASN
1	A	85	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	302	ASN
1	A	310	GLN
1	A	321	ASN
1	A	370	GLN
1	A	384	HIS
1	A	386	GLN
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	491	GLN
1	A	492	ASN
1	A	517	ASN
1	A	549	GLN
1	A	550	GLN
1	A	557	ASN
1	A	560	ASN

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

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.

No monomer is involved in short contacts.

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^{th} 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^2)	Q<0.9
1	A	548/584 (93%)	0.73	67 (12%) 10 6	3, 14, 44, 78	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	299	GLY	9.1
1	A	340	ALA	7.6
1	A	228	THR	5.5
1	A	562	VAL	5.4
1	A	514	ALA	5.0
1	A	157	ALA	4.7
1	A	226	SER	4.6
1	A	492	ASN	4.6
1	A	116	ALA	4.6
1	A	486	ALA	4.5
1	A	154	SER	4.0
1	A	515	SER	4.0
1	A	194	THR	3.9
1	A	276	THR	3.8
1	A	394	THR	3.6
1	A	245	THR	3.5
1	A	147	ASN	3.4
1	A	399	THR	3.4
1	A	517	ASN	3.4
1	A	289	PRO	3.3
1	A	182	THR	3.2
1	A	156	SER	3.2
1	A	513	ASP	3.1
1	A	260	GLU	3.1
1	A	124	GLY	3.1
1	A	360	GLY	3.1
1	A	179	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	401	ILE	3.0
1	A	237	ASP	3.0
1	A	225	THR	3.0
1	A	75	GLU	2.9
1	A	365	GLN	2.9
1	A	516	ALA	2.9
1	A	477	ASP	2.9
1	A	163	LYS	2.8
1	A	86	ASN	2.8
1	A	56	ASN	2.6
1	A	357	ILE	2.6
1	A	47	ASN	2.6
1	A	168	ASP	2.6
1	A	241	VAL	2.5
1	A	181	ASN	2.5
1	A	45	PHE	2.4
1	A	367	ASP	2.4
1	A	536	LYS	2.4
1	A	131	ASN	2.4
1	A	334	ALA	2.3
1	A	312	LYS	2.3
1	A	326	THR	2.3
1	A	65	SER	2.3
1	A	373	ASP	2.2
1	A	436	ILE	2.2
1	A	427	ASP	2.2
1	A	511	ASP	2.2
1	A	161	PRO	2.2
1	A	114	ALA	2.2
1	A	159	GLN	2.2
1	A	370	GLN	2.2
1	A	337	GLY	2.1
1	A	46	ASN	2.1
1	A	366	THR	2.1
1	A	519	SER	2.1
1	A	220	PRO	2.1
1	A	500	VAL	2.1
1	A	501	LYS	2.0
1	A	493	ASN	2.0
1	A	379	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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. The B-factors column lists the minimum, median, 95^{th} 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	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CA	A	585	1/1	0.90	0.13	30,30,30,30	1

6.5 Other polymers (i)

There are no such residues in this entry.