Full wwPDB X-ray Structure Validation Report ⓘ

Apr 11, 2023 – 12:07 AM EDT

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 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:

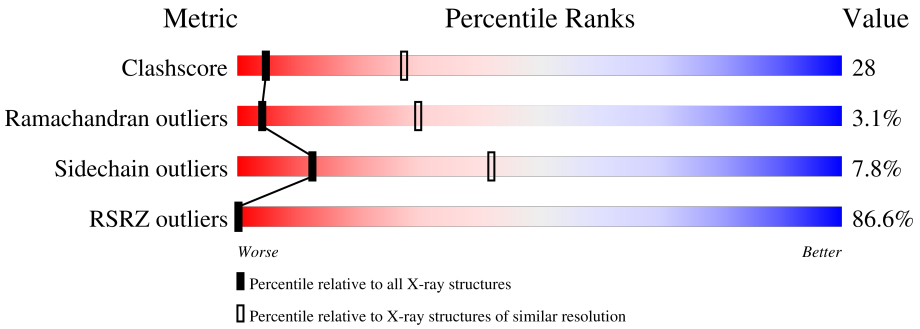
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 3.50 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)
RSRZ outliers	127900	1559 (3.60-3.40)

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	81% 51% 36% 7% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CA	A	585	-	-	-	X
2	CA	A	586	-	-	-	X

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4321 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
1	A	544	Total	C	N	O	S	0	0	0
			4319	2745	737	821	16			

There is a discrepancy between the modelled and reference sequences:

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

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

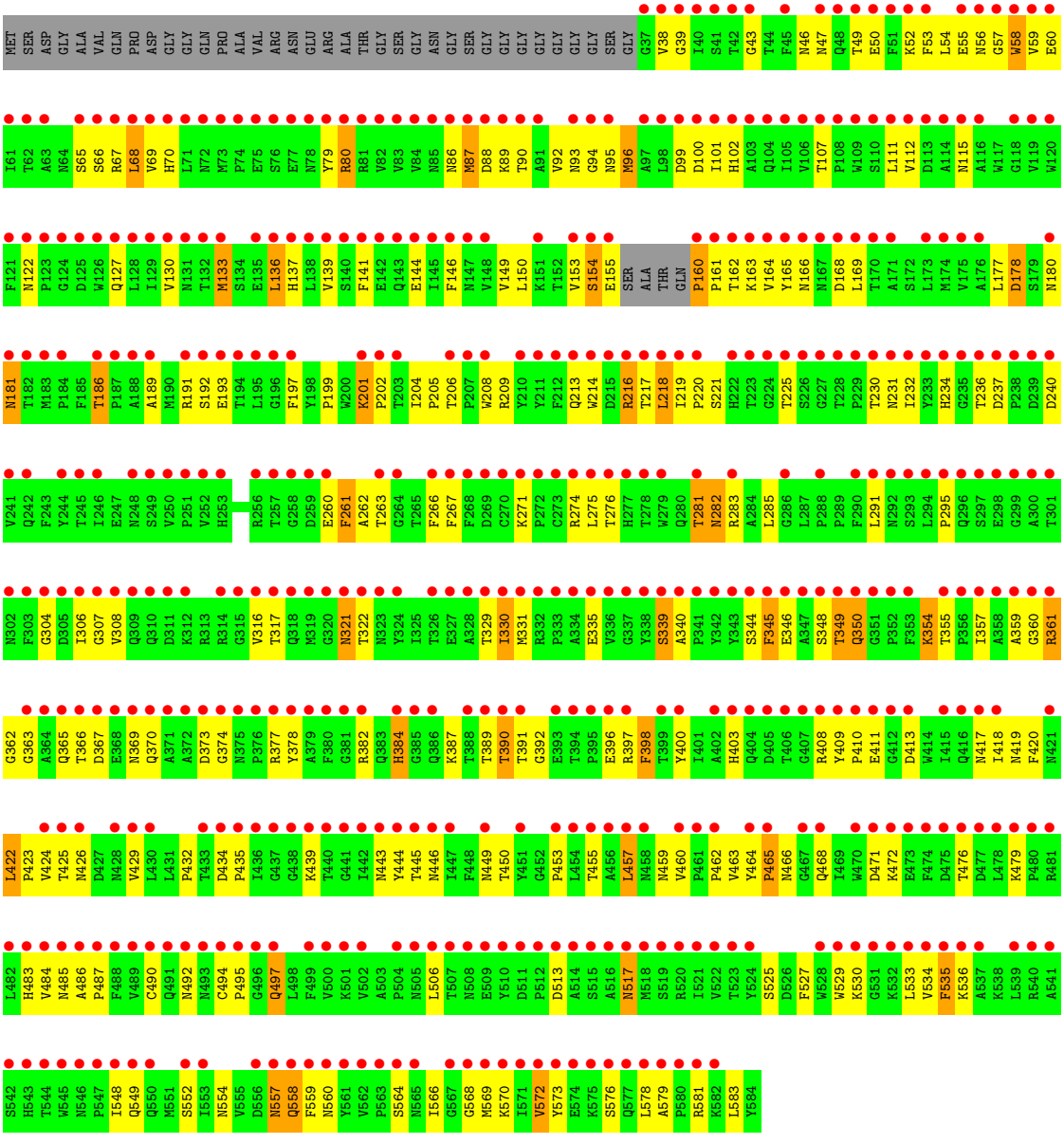
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		

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	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
$< I/\sigma(I) >$ [1]	1457.89 (at 3.52Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.260 , (Not available) 0.325 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	30.3	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.51 , 42.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.35$, $< L^2 > = 0.17$	Xtriage
Estimated twinning fraction	0.169 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.17	EDS
Total number of atoms	4321	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[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	0.54	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(^{o})	Ideal(^{o})
1	A	58	TRP	N-CA-C	-5.17	97.04	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 Too-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 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	4319	0	4118	236	0
2	A	2	0	0	0	0
All	All	4321	0	4118	236	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 28.

All (236) 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:366:THR:HA	1:A:370:GLN:HB2	1.24	1.19
1:A:360:GLY:HA2	1:A:374:GLY:HA3	1.36	1.06
1:A:155:GLU:HB3	1:A:160:PRO:HA	1.44	0.98
1:A:160:PRO:HB2	1:A:161:PRO:CD	1.95	0.96
1:A:160:PRO:HB2	1:A:161:PRO:HD3	1.47	0.94
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:361:ARG:HG2	1:A:362:GLY:H	1.39	0.87
1:A:349:THR:HG22	1:A:350:GLN:HG3	1.56	0.87
1:A:154:SER:HB2	1:A:164:VAL:HG22	1.56	0.86
1:A:422:LEU:H	1:A:422:LEU:HD23	1.39	0.86
1:A:366:THR:HA	1:A:370:GLN:CB	2.05	0.86
1:A:554:ASN:H	1:A:557:ASN:ND2	1.74	0.84
1:A:557:ASN:HD22	1:A:558:GLN:N	1.76	0.84
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:139:VAL:HB	1:A:534:VAL:O	1.83	0.78
1:A:52:LYS:HG2	1:A:54:LEU:HD21	1.66	0.77
1:A:560:ASN:HB3	1:A:572:VAL:HG21	1.67	0.77
1:A:96:MET:HG2	1:A:220:PRO:HA	1.67	0.76
1:A:360:GLY:HA2	1:A:374:GLY:CA	2.16	0.75
1:A:554:ASN:N	1:A:557:ASN:HD21	1.79	0.75
1:A:155:GLU:HB3	1:A:160:PRO:CA	2.16	0.75
1:A:38:VAL:HG21	1:A:169:LEU:HD13	1.67	0.74
1:A:410:PRO:HA	1:A:413:ASP:OD2	1.87	0.74
1:A:322:THR:HG21	1:A:420:PHE:CD2	2.22	0.74
1:A:560:ASN:HB3	1:A:572:VAL:CG2	2.18	0.73
1:A:154:SER:O	1:A:163:LYS:HA	1.91	0.71
1:A:180:ASN:O	1:A:181:ASN:HB2	1.90	0.71
1:A:557:ASN:HD22	1:A:558:GLN:H	1.36	0.70
1:A:408:ARG:HG3	1:A:408:ARG:HH11	1.56	0.69
1:A:67:ARG:HG2	1:A:67:ARG:HH11	1.57	0.69
1:A:219:ILE:HG23	1:A:220:PRO:HD2	1.74	0.69
1:A:322:THR:CG2	1:A:420:PHE:HD2	2.04	0.69
1:A:160:PRO:CB	1:A:161:PRO:CD	2.72	0.68
1:A:221:SER:HB2	1:A:225:THR:HG21	1.74	0.67
1:A:316:VAL:O	1:A:330:ILE:HD12	1.95	0.67
1:A:361:ARG:HG2	1:A:362:GLY:N	2.10	0.66
1:A:43:GLY:HA3	1:A:146:PHE:CD2	2.30	0.66
1:A:366:THR:O	1:A:370:GLN:HG2	1.96	0.66
1:A:92:VAL:O	1:A:93:ASN:HB2	1.97	0.65
1:A:69:VAL:HG13	1:A:205:PRO:HD3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ASP:OD1	1:A:216:ARG:NH2	2.30	0.64
1:A:330:ILE:HG13	1:A:331:MET:N	2.12	0.64
1:A:213:GLN:HG3	1:A:240:ASP:CB	2.28	0.64
1:A:339:SER:O	1:A:449:ASN:HA	1.98	0.63
1:A:68:LEU:HG	1:A:68:LEU:O	1.98	0.63
1:A:58:TRP:CE3	1:A:536:LYS:HE3	2.34	0.62
1:A:94:GLY:HA2	1:A:221:SER:O	1.98	0.62
1:A:107:THR:HG1	1:A:208:TRP:HE3	1.47	0.62
1:A:464:TYR:CE2	1:A:465:PRO:HB3	2.35	0.61
1:A:154:SER:HB2	1:A:164:VAL:CG2	2.29	0.61
1:A:422:LEU:H	1:A:422:LEU:CD2	2.13	0.61
1:A:460:VAL:HG11	1:A:484:VAL:HA	1.83	0.61
1:A:193:GLU:CB	1:A:206:THR:HG21	2.31	0.60
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:317:THR:HG22	1:A:330:ILE:HA	1.84	0.60
1:A:361:ARG:CG	1:A:362:GLY:H	2.08	0.60
1:A:47:ASN:OD1	1:A:66:SER:N	2.29	0.60
1:A:70:HIS:O	1:A:204:ILE:HG22	2.01	0.60
1:A:87:MET:HG3	1:A:231:ASN:ND2	2.17	0.60
1:A:160:PRO:C	1:A:162:THR:H	2.05	0.59
1:A:79:TYR:CE2	1:A:107:THR:HG22	2.37	0.59
1:A:55:GLU:O	1:A:56:ASN:HB2	2.02	0.59
1:A:354:LYS:HD2	1:A:355:THR:N	2.17	0.59
1:A:38:VAL:HG12	1:A:39:GLY:N	2.18	0.58
1:A:68:LEU:O	1:A:68:LEU:CG	2.51	0.58
1:A:354:LYS:HD2	1:A:355:THR:H	1.68	0.58
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:47:ASN:ND2	1:A:199:PRO:HB3	2.19	0.58
1:A:282:ASN:OD1	1:A:335:GLU:HA	2.03	0.58
1:A:366:THR:CA	1:A:370:GLN:HB2	2.15	0.58
1:A:115:ASN:OD1	1:A:468:GLN:HG2	2.04	0.58
1:A:361:ARG:HG2	1:A:366:THR:HG21	1.86	0.57
1:A:281:THR:O	1:A:283:ARG:N	2.37	0.57
1:A:560:ASN:CB	1:A:572:VAL:HG21	2.34	0.57
1:A:197:PHE:CE2	1:A:384:HIS:HB3	2.40	0.57
1:A:69:VAL:HB	1:A:527:PHE:CE1	2.40	0.56
1:A:536:LYS:HG2	1:A:536:LYS:O	2.04	0.56
1:A:49:THR:C	1:A:50:GLU:HG3	2.24	0.56
1:A:107:THR:HG21	1:A:208:TRP:CZ3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:PRO:HD3	1:A:573:TYR:HA	1.87	0.56
1:A:38:VAL:CG2	1:A:169:LEU:HD13	2.35	0.56
1:A:348:SER:O	1:A:350:GLN:N	2.38	0.56
1:A:193:GLU:CG	1:A:206:THR:HG21	2.35	0.56
1:A:295:PRO:HD3	1:A:304:GLY:CA	2.36	0.56
1:A:346:GLU:HG3	1:A:355:THR:OG1	2.06	0.56
1:A:357:ILE:HG22	1:A:359:ALA:H	1.70	0.56
1:A:398:PHE:HE1	1:A:400:TYR:HB2	1.71	0.55
1:A:67:ARG:HG2	1:A:67:ARG:NH1	2.16	0.55
1:A:361:ARG:NE	1:A:366:THR:HG22	2.22	0.55
1:A:457:LEU:N	1:A:457:LEU:HD23	2.22	0.55
1:A:59:VAL:HG12	1:A:60:GLU:N	2.21	0.55
1:A:330:ILE:HG13	1:A:331:MET:H	1.71	0.55
1:A:52:LYS:HD3	1:A:60:GLU:OE2	2.07	0.55
1:A:197:PHE:CE2	1:A:465:PRO:O	2.59	0.55
1:A:396:GLU:HA	1:A:396:GLU:OE1	2.07	0.54
1:A:408:ARG:HG3	1:A:408:ARG:NH1	2.20	0.54
1:A:361:ARG:HE	1:A:366:THR:HG22	1.71	0.54
1:A:465:PRO:HD2	1:A:466:ASN:ND2	2.22	0.54
1:A:409:TYR:CE2	1:A:411:GLU:HB2	2.42	0.54
1:A:160:PRO:O	1:A:162:THR:N	2.41	0.54
1:A:387:LYS:O	1:A:390:THR:HB	2.07	0.54
1:A:47:ASN:OD1	1:A:65:SER:HA	2.08	0.54
1:A:340:ALA:HB3	1:A:357:ILE:HD12	1.89	0.54
1:A:261:PHE:CD1	1:A:261:PHE:C	2.81	0.53
1:A:317:THR:HG21	1:A:329:THR:HG22	1.90	0.53
1:A:557:ASN:ND2	1:A:557:ASN:H	2.05	0.53
1:A:422:LEU:CD2	1:A:422:LEU:N	2.72	0.53
1:A:557:ASN:O	1:A:559:PHE:N	2.41	0.53
1:A:403:HIS:CD2	1:A:549:GLN:HE22	2.27	0.53
1:A:219:ILE:HG12	1:A:230:THR:OG1	2.08	0.52
1:A:363:GLY:HA3	1:A:365:GLN:NE2	2.23	0.52
1:A:535:PHE:CD1	1:A:535:PHE:N	2.78	0.52
1:A:99:ASP:CG	1:A:216:ARG:HH21	2.14	0.52
1:A:86:ASN:ND2	1:A:100:ASP:HB2	2.25	0.51
1:A:111:LEU:HD12	1:A:112:VAL:N	2.25	0.51
1:A:557:ASN:ND2	1:A:558:GLN:N	2.53	0.51
1:A:65:SER:O	1:A:530:LYS:HA	2.10	0.51
1:A:219:ILE:CG2	1:A:220:PRO:HD2	2.38	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	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:GLU:HA	1:A:262:ALA:HA	1.93	0.51
1:A:150:LEU:HG	1:A:525:SER:HB2	1.92	0.51
1:A:276:THR:OG1	1:A:581:ARG:HD3	2.11	0.51
1:A:101:ILE:O	1:A:102:HIS:HB3	2.11	0.50
1:A:80:ARG:NH1	1:A:80:ARG:HG2	2.25	0.50
1:A:361:ARG:CG	1:A:362:GLY:N	2.71	0.50
1:A:59:VAL:HG21	1:A:133:MET:HE2	1.93	0.50
1:A:52:LYS:HE2	1:A:54:LEU:HD21	1.93	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: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:476:THR:O	1:A:479:LYS:HE2	2.12	0.49
1:A:232:ILE:HD11	1:A:234:HIS:CE1	2.48	0.49
1:A:122:ASN:OD1	1:A:122:ASN:C	2.51	0.49
1:A:217:THR:HG22	1:A:218:LEU:N	2.28	0.49
1:A:422:LEU:HD23	1:A:422:LEU:N	2.15	0.48
1:A:322:THR:CG2	1:A:420:PHE:CD2	2.91	0.48
1:A:366:THR:HA	1:A:370:GLN:CG	2.43	0.48
1:A:564:SER:C	1:A:566:ILE:H	2.16	0.48
1:A:68:LEU:C	1:A:68:LEU:HD12	2.33	0.47
1:A:533:LEU:HG	1:A:535:PHE:CE1	2.48	0.47
1:A:160:PRO:HB2	1:A:161:PRO:HD2	1.93	0.47
1:A:472:LYS:HA	1:A:494:CYS:SG	2.54	0.47
1:A:267:PHE:N	1:A:267:PHE:CD1	2.83	0.47
1:A:462:PRO:HD2	1:A:576:SER:OG	2.15	0.47
1:A:53:PHE:O	1:A:54:LEU:HD23	2.15	0.47
1:A:177:LEU:HD22	1:A:263:THR:HG22	1.96	0.47
1:A:214:TRP:O	1:A:350:GLN:HG2	2.15	0.47
1:A:136:LEU:C	1:A:137:HIS:HD2	2.19	0.47
1:A:155:GLU:CB	1:A:160:PRO:HA	2.31	0.46
1:A:189:ALA:HB3	1:A:468:GLN:HG3	1.98	0.46
1:A:201:LYS:HG3	1:A:202:PRO:O	2.15	0.46
1:A:367:ASP:C	1:A:369:ASN:H	2.19	0.46
1:A:186:THR:O	1:A:186:THR:OG1	2.29	0.46
1:A:378:TYR:O	1:A:397:ARG:HA	2.15	0.46
1:A:425:THR:HG22	1:A:426:ASN:N	2.30	0.46
1:A:424:VAL:CG2	1:A:429:VAL:HB	2.46	0.46
1:A:557:ASN:HD22	1:A:557:ASN:N	2.12	0.46
1:A:66:SER:HA	1:A:529:TRP:O	2.15	0.45
1:A:236:THR:HG22	1:A:237:ASP:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:PHE:CD1	1:A:495:PRO:HG3	2.51	0.45
1:A:424:VAL:HG21	1:A:429:VAL:HB	1.97	0.45
1:A:497:GLN:HE21	1:A:497:GLN:HB2	1.63	0.45
1:A:79:TYR:CD2	1:A:107:THR:HG22	2.52	0.45
1:A:144:GLU:HB3	1:A:262:ALA:CB	2.47	0.45
1:A:557:ASN:ND2	1:A:557:ASN:N	2.64	0.45
1:A:398:PHE:CD1	1:A:398:PHE:C	2.90	0.45
1:A:149:VAL:C	1:A:150:LEU:HD12	2.37	0.45
1:A:443:ASN:OD1	1:A:445:THR:N	2.50	0.45
1:A:455:THR:HG22	1:A:457:LEU:CD2	2.47	0.45
1:A:494:CYS:O	1:A:495:PRO:C	2.55	0.45
1:A:49:THR:CG2	1:A:50:GLU:N	2.80	0.44
1:A:66:SER:O	1:A:67:ARG:NH1	2.49	0.44
1:A:218:LEU:HD12	1:A:219:ILE:N	2.32	0.44
1:A:345:PHE:N	1:A:345:PHE:HD1	2.15	0.44
1:A:548:ILE:CD1	1:A:579:ALA:HB2	2.47	0.44
1:A:177:LEU:C	1:A:177:LEU:HD12	2.37	0.44
1:A:221:SER:HB2	1:A:225:THR:CG2	2.45	0.44
1:A:365:GLN:O	1:A:370:GLN:HG3	2.18	0.44
1:A:486:ALA:HA	1:A:487:PRO:HD3	1.81	0.44
1:A:583:LEU:C	1:A:583:LEU:HD23	2.38	0.44
1:A:377:ARG:HG3	1:A:377:ARG:HH11	1.83	0.44
1:A:69:VAL:CG1	1:A:205:PRO:HD3	2.48	0.43
1:A:153:VAL:HG22	1:A:165:TYR:CD1	2.53	0.43
1:A:127:GLN:NE2	1:A:552:SER:HA	2.33	0.43
1:A:46:ASN:OD1	1:A:46:ASN:C	2.54	0.43
1:A:398:PHE:HE2	1:A:466:ASN:ND2	2.16	0.43
1:A:90:THR:CG2	1:A:99:ASP:HA	2.48	0.43
1:A:218:LEU:HD12	1:A:218:LEU:C	2.39	0.43
1:A:86:ASN:O	1:A:87:MET:C	2.55	0.43
1:A:295:PRO:HD3	1:A:304:GLY:HA2	2.00	0.43
1:A:434:ASP:HA	1:A:435:PRO:HD3	1.73	0.42
1:A:191:ARG:O	1:A:192:SER:C	2.57	0.42
1:A:417:ASN:OD1	1:A:419:ASN:ND2	2.50	0.42
1:A:80:ARG:HH11	1:A:80:ARG:CG	2.32	0.42
1:A:389:THR:HG23	1:A:568:GLY:HA2	2.02	0.42
1:A:391:THR:C	1:A:392:GLY:O	2.58	0.42
1:A:464:TYR:CD2	1:A:465:PRO:HB3	2.55	0.42
1:A:107:THR:HG21	1:A:208:TRP:CE3	2.54	0.42
1:A:471:ASP:OD2	1:A:483:HIS:ND1	2.51	0.42
1:A:217:THR:CG2	1:A:218:LEU:N	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:PRO:HB3	1:A:439:LYS:O	2.19	0.42
1:A:43:GLY:CA	1:A:146:PHE:CD2	3.01	0.42
1:A:564:SER:O	1:A:566:ILE:N	2.53	0.42
1:A:400:TYR:CD2	1:A:463:VAL:HG13	2.55	0.42
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:59:VAL:HG21	1:A:133:MET:CE	2.50	0.41
1:A:80:ARG:HG2	1:A:80:ARG:HH11	1.85	0.41
1:A:291:LEU:HA	1:A:306:ILE:HA	2.01	0.41
1:A:90:THR:HG21	1:A:99:ASP:HA	2.02	0.41
1:A:339:SER:HB2	1:A:450:THR:OG1	2.20	0.41
1:A:439:LYS:HA	1:A:439:LYS:HD3	1.74	0.41
1:A:506:LEU:H	1:A:506:LEU:HG	1.68	0.41
1:A:569:MET:HE3	1:A:570:LYS:H	1.84	0.41
1:A:89:LYS:HE2	1:A:89:LYS:HB2	1.86	0.41
1:A:424:VAL:O	1:A:424:VAL:HG13	2.20	0.41
1:A:459:ASN:OD1	1:A:460:VAL:HG22	2.19	0.41
1:A:307:GLY:C	1:A:308:VAL:HG23	2.41	0.41
1:A:354:LYS:NZ	1:A:373:ASP:OD1	2.50	0.41
1:A:274:ARG:O	1:A:275:LEU:HD23	2.21	0.41
1:A:321:ASN:HD22	1:A:321:ASN:H	1.68	0.41
1:A:389:THR:HG23	1:A:568:GLY:CA	2.51	0.41
1:A:459:ASN:OD1	1:A:460:VAL:N	2.54	0.41
1:A:144:GLU:CB	1:A:262:ALA:HA	2.52	0.41
1:A:377:ARG:HG3	1:A:377:ARG:NH1	2.36	0.40
1:A:382:ARG:NH2	1:A:392:GLY:O	2.54	0.40
1:A:130:VAL:CG1	1:A:578:LEU:HD22	2.52	0.40
1:A:382:ARG:NH1	1:A:382:ARG:HG3	2.37	0.40
1:A:483:HIS:HB3	1:A:485:ASN:OD1	2.22	0.40
1:A:517:ASN:HD22	1:A:517:ASN:HA	1.59	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	542/584 (93%)	455 (84%)	70 (13%)	17 (3%)	4 30

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	ASN
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 (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	473/495 (96%)	436 (92%)	37 (8%)	12 42

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

Mol	Chain	Res	Type
1	A	68	LEU
1	A	80	ARG

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Mol	Chain	Res	Type
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
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

Sometimes 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

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

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.

No monomer is involved in short contacts.

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

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	544/584 (93%)	3.76	471 (86%)	0	0	9, 32, 71, 100	0

All (471) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	351	GLY	12.2
1	A	224	GLY	11.2
1	A	475	ASP	10.3
1	A	37	GLY	9.8
1	A	381	GLY	8.8
1	A	560	ASN	8.8
1	A	235	GLY	8.8
1	A	226	SER	8.7
1	A	269	ASP	8.5
1	A	270	CYS	8.5
1	A	39	GLY	8.3
1	A	160	PRO	8.2
1	A	360	GLY	8.1
1	A	196	GLY	8.1
1	A	544	THR	8.1
1	A	394	THR	8.0
1	A	492	ASN	7.8
1	A	412	GLY	7.7
1	A	227	GLY	7.7
1	A	417	ASN	7.6
1	A	477	ASP	7.4
1	A	352	PRO	7.2
1	A	225	THR	7.2
1	A	565	ASN	7.2
1	A	517	ASN	7.2
1	A	307	GLY	7.1
1	A	38	VAL	7.0

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Mol	Chain	Res	Type	RSRZ
1	A	52	LYS	7.0
1	A	155	GLU	7.0
1	A	523	THR	7.0
1	A	365	GLN	6.9
1	A	343	TYR	6.9
1	A	336	VAL	6.9
1	A	319	MET	6.9
1	A	91	ALA	6.9
1	A	572	VAL	6.9
1	A	218	LEU	6.9
1	A	166	ASN	6.8
1	A	135	GLU	6.8
1	A	183	MET	6.8
1	A	273	CYS	6.7
1	A	217	THR	6.7
1	A	192	SER	6.7
1	A	426	ASN	6.6
1	A	550	GLN	6.6
1	A	100	ASP	6.5
1	A	213	GLN	6.5
1	A	388	THR	6.5
1	A	435	PRO	6.5
1	A	371	ALA	6.4
1	A	167	ASN	6.4
1	A	543	HIS	6.3
1	A	363	GLY	6.3
1	A	140	SER	6.2
1	A	182	THR	6.2
1	A	88	ASP	6.1
1	A	108	PRO	6.1
1	A	90	THR	6.0
1	A	322	THR	6.0
1	A	537	ALA	6.0
1	A	520	ARG	6.0
1	A	259	ASP	6.0
1	A	72	ASN	6.0
1	A	441	GLY	5.9
1	A	434	ASP	5.8
1	A	244	TYR	5.8
1	A	310	GLN	5.8
1	A	547	PRO	5.8
1	A	445	THR	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	86	ASN	5.7
1	A	118	GLY	5.7
1	A	531	GLY	5.7
1	A	85	ASN	5.7
1	A	358	ALA	5.7
1	A	407	GLY	5.6
1	A	223	THR	5.6
1	A	399	THR	5.6
1	A	410	PRO	5.6
1	A	203	THR	5.6
1	A	568	GLY	5.5
1	A	234	HIS	5.5
1	A	493	ASN	5.5
1	A	513	ASP	5.5
1	A	438	GLY	5.5
1	A	514	ALA	5.5
1	A	320	GLY	5.4
1	A	542	SER	5.4
1	A	377	ARG	5.4
1	A	474	PHE	5.4
1	A	359	ALA	5.4
1	A	248	ASN	5.3
1	A	286	GLY	5.3
1	A	114	ALA	5.3
1	A	425	THR	5.3
1	A	137	HIS	5.3
1	A	105	ILE	5.2
1	A	556	ASP	5.2
1	A	301	THR	5.2
1	A	139	VAL	5.2
1	A	346	GLU	5.2
1	A	428	ASN	5.1
1	A	193	GLU	5.1
1	A	403	HIS	5.1
1	A	364	ALA	5.1
1	A	194	THR	5.1
1	A	154	SER	5.1
1	A	389	THR	5.1
1	A	94	GLY	5.0
1	A	206	THR	5.0
1	A	541	ALA	5.0
1	A	251	PRO	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	374	GLY	4.9
1	A	461	PRO	4.9
1	A	144	GLU	4.9
1	A	48	GLN	4.9
1	A	240	ASP	4.9
1	A	491	GLN	4.9
1	A	366	THR	4.9
1	A	242	GLN	4.9
1	A	443	ASN	4.9
1	A	455	THR	4.9
1	A	561	TYR	4.9
1	A	161	PRO	4.8
1	A	323	ASN	4.8
1	A	170	THR	4.8
1	A	263	THR	4.8
1	A	71	LEU	4.8
1	A	260	GLU	4.7
1	A	519	SER	4.7
1	A	324	TYR	4.7
1	A	546	ASN	4.7
1	A	101	ILE	4.7
1	A	195	LEU	4.7
1	A	386	GLN	4.6
1	A	122	ASN	4.6
1	A	272	PRO	4.6
1	A	370	GLN	4.6
1	A	536	LYS	4.6
1	A	344	SER	4.6
1	A	98	LEU	4.6
1	A	376	PRO	4.5
1	A	232	ILE	4.5
1	A	582	LYS	4.5
1	A	494	CYS	4.5
1	A	237	ASP	4.5
1	A	65	SER	4.5
1	A	569	MET	4.5
1	A	302	ASN	4.5
1	A	328	ALA	4.4
1	A	480	PRO	4.4
1	A	62	THR	4.4
1	A	104	GLN	4.4
1	A	186	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	236	THR	4.4
1	A	390	THR	4.4
1	A	486	ALA	4.4
1	A	202	PRO	4.4
1	A	97	ALA	4.4
1	A	391	THR	4.3
1	A	187	PRO	4.3
1	A	58	TRP	4.3
1	A	184	PRO	4.3
1	A	268	PHE	4.3
1	A	458	ASN	4.3
1	A	222	HIS	4.3
1	A	557	ASN	4.3
1	A	238	PRO	4.3
1	A	78	ASN	4.3
1	A	327	GLU	4.3
1	A	437	GLY	4.3
1	A	375	ASN	4.2
1	A	63	ALA	4.2
1	A	145	ILE	4.2
1	A	413	ASP	4.2
1	A	121	PHE	4.2
1	A	181	ASN	4.2
1	A	293	SER	4.2
1	A	483	HIS	4.2
1	A	532	LYS	4.2
1	A	357	ILE	4.2
1	A	356	PRO	4.2
1	A	81	ARG	4.2
1	A	125	ASP	4.2
1	A	524	TYR	4.2
1	A	506	LEU	4.2
1	A	559	PHE	4.2
1	A	367	ASP	4.2
1	A	297	SER	4.1
1	A	296	GLN	4.1
1	A	214	TRP	4.1
1	A	231	ASN	4.1
1	A	341	PRO	4.1
1	A	229	PRO	4.1
1	A	212	PHE	4.1
1	A	326	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	210	TYR	4.1
1	A	553	ILE	4.0
1	A	153	VAL	4.0
1	A	99	ASP	4.0
1	A	228	THR	4.0
1	A	115	ASN	4.0
1	A	456	ALA	4.0
1	A	129	ILE	4.0
1	A	132	THR	4.0
1	A	372	ALA	4.0
1	A	500	VAL	4.0
1	A	564	SER	4.0
1	A	55	GLU	3.9
1	A	257	THR	3.9
1	A	318	GLN	3.9
1	A	505	ASN	3.9
1	A	258	GLY	3.9
1	A	529	TRP	3.9
1	A	56	ASN	3.9
1	A	457	LEU	3.9
1	A	130	VAL	3.8
1	A	451	TYR	3.8
1	A	288	PRO	3.8
1	A	314	ARG	3.8
1	A	175	VAL	3.8
1	A	411	GLU	3.8
1	A	349	THR	3.8
1	A	577	GLN	3.8
1	A	147	ASN	3.8
1	A	396	GLU	3.8
1	A	103	ALA	3.8
1	A	230	THR	3.8
1	A	281	THR	3.8
1	A	208	TRP	3.8
1	A	348	SER	3.8
1	A	518	MET	3.8
1	A	67	ARG	3.8
1	A	581	ARG	3.8
1	A	57	GLY	3.8
1	A	70	HIS	3.8
1	A	496	GLY	3.7
1	A	164	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	402	ALA	3.7
1	A	511	ASP	3.7
1	A	444	TYR	3.7
1	A	416	GLN	3.7
1	A	539	LEU	3.7
1	A	331	MET	3.7
1	A	68	LEU	3.7
1	A	163	LYS	3.7
1	A	409	TYR	3.7
1	A	545	TRP	3.7
1	A	510	TYR	3.7
1	A	488	PHE	3.7
1	A	165	TYR	3.6
1	A	563	PRO	3.6
1	A	80	ARG	3.6
1	A	295	PRO	3.6
1	A	124	GLY	3.6
1	A	252	VAL	3.6
1	A	369	ASN	3.6
1	A	298	GLU	3.6
1	A	141	PHE	3.6
1	A	395	PRO	3.6
1	A	279	TRP	3.6
1	A	338	TYR	3.6
1	A	404	GLN	3.6
1	A	113	ASP	3.6
1	A	60	GLU	3.6
1	A	478	LEU	3.6
1	A	484	VAL	3.6
1	A	191	ARG	3.6
1	A	87	MET	3.5
1	A	429	VAL	3.5
1	A	504	PRO	3.5
1	A	406	THR	3.5
1	A	315	GLY	3.5
1	A	571	ILE	3.5
1	A	373	ASP	3.5
1	A	485	ASN	3.5
1	A	51	PHE	3.5
1	A	173	LEU	3.5
1	A	436	ILE	3.5
1	A	574	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	120	TRP	3.5
1	A	309	GLN	3.5
1	A	558	GLN	3.5
1	A	439	LYS	3.5
1	A	211	TYR	3.5
1	A	509	GLU	3.5
1	A	347	ALA	3.4
1	A	345	PHE	3.4
1	A	530	LYS	3.4
1	A	442	ILE	3.4
1	A	197	PHE	3.4
1	A	146	PHE	3.4
1	A	102	HIS	3.4
1	A	418	ILE	3.4
1	A	340	ALA	3.4
1	A	271	LYS	3.4
1	A	311	ASP	3.4
1	A	393	GLU	3.4
1	A	253	HIS	3.3
1	A	379	ALA	3.3
1	A	143	GLN	3.3
1	A	93	ASN	3.3
1	A	497	GLN	3.3
1	A	521	ILE	3.3
1	A	408	ARG	3.3
1	A	317	THR	3.3
1	A	329	THR	3.3
1	A	467	GLY	3.3
1	A	169	LEU	3.3
1	A	73	MET	3.2
1	A	533	LEU	3.2
1	A	303	PHE	3.2
1	A	201	LYS	3.2
1	A	111	LEU	3.2
1	A	168	ASP	3.2
1	A	400	TYR	3.2
1	A	95	ASN	3.2
1	A	305	ASP	3.2
1	A	304	GLY	3.2
1	A	424	VAL	3.2
1	A	465	PRO	3.2
1	A	45	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	549	GLN	3.2
1	A	382	ARG	3.2
1	A	119	VAL	3.2
1	A	512	PRO	3.2
1	A	580	PRO	3.2
1	A	219	ILE	3.2
1	A	245	THR	3.1
1	A	180	ASN	3.1
1	A	291	LEU	3.1
1	A	339	SER	3.1
1	A	40	ILE	3.1
1	A	274	ARG	3.1
1	A	528	TRP	3.1
1	A	138	LEU	3.1
1	A	249	SER	3.1
1	A	112	VAL	3.1
1	A	308	VAL	3.1
1	A	507	THR	3.1
1	A	502	VAL	3.0
1	A	220	PRO	3.0
1	A	508	ASN	3.0
1	A	355	THR	3.0
1	A	239	ASP	3.0
1	A	49	THR	3.0
1	A	440	THR	3.0
1	A	148	VAL	3.0
1	A	136	LEU	3.0
1	A	576	SER	3.0
1	A	292	ASN	3.0
1	A	290	PHE	3.0
1	A	361	ARG	2.9
1	A	246	ILE	2.9
1	A	300	ALA	2.9
1	A	142	GLU	2.9
1	A	276	THR	2.9
1	A	397	ARG	2.9
1	A	353	PHE	2.9
1	A	384	HIS	2.9
1	A	482	LEU	2.9
1	A	449	ASN	2.9
1	A	174	MET	2.9
1	A	109	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	277	HIS	2.8
1	A	570	LYS	2.8
1	A	110	SER	2.8
1	A	75	GLU	2.8
1	A	468	GLN	2.8
1	A	335	GLU	2.8
1	A	405	ASP	2.8
1	A	127	GLN	2.8
1	A	535	PHE	2.8
1	A	107	THR	2.8
1	A	171	ALA	2.8
1	A	332	ARG	2.8
1	A	471	ASP	2.8
1	A	501	LYS	2.8
1	A	470	TRP	2.7
1	A	489	VAL	2.7
1	A	264	GLY	2.7
1	A	342	TYR	2.7
1	A	89	LYS	2.7
1	A	567	GLY	2.7
1	A	447	ILE	2.7
1	A	464	TYR	2.7
1	A	415	ILE	2.7
1	A	495	PRO	2.6
1	A	256	ARG	2.6
1	A	74	PRO	2.6
1	A	233	TYR	2.6
1	A	487	PRO	2.6
1	A	368	GLU	2.6
1	A	462	PRO	2.6
1	A	66	SER	2.6
1	A	128	LEU	2.6
1	A	481	ARG	2.5
1	A	42	THR	2.5
1	A	283	ARG	2.5
1	A	43	GLY	2.5
1	A	337	GLY	2.5
1	A	578	LEU	2.5
1	A	350	GLN	2.5
1	A	82	VAL	2.5
1	A	50	GLU	2.5
1	A	299	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	575	LYS	2.4
1	A	69	VAL	2.4
1	A	77	GLU	2.4
1	A	454	LEU	2.4
1	A	126	TRP	2.4
1	A	123	PRO	2.4
1	A	84	VAL	2.4
1	A	216	ARG	2.4
1	A	385	GLY	2.4
1	A	380	PHE	2.4
1	A	312	LYS	2.4
1	A	83	VAL	2.4
1	A	306	ILE	2.3
1	A	460	VAL	2.3
1	A	316	VAL	2.3
1	A	266	PHE	2.3
1	A	421	ASN	2.3
1	A	430	LEU	2.3
1	A	133	MET	2.3
1	A	472	LYS	2.3
1	A	490	CYS	2.3
1	A	41	SER	2.3
1	A	540	ARG	2.3
1	A	189	ALA	2.3
1	A	61	ILE	2.3
1	A	241	VAL	2.3
1	A	275	LEU	2.3
1	A	515	SER	2.3
1	A	516	ALA	2.2
1	A	79	TYR	2.2
1	A	522	VAL	2.2
1	A	433	THR	2.2
1	A	278	THR	2.2
1	A	176	ALA	2.2
1	A	548	ILE	2.2
1	A	552	SER	2.2
1	A	453	PRO	2.2
1	A	47	ASN	2.2
1	A	207	PRO	2.2
1	A	330	ILE	2.2
1	A	151	LYS	2.1
1	A	562	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	53	PHE	2.1
1	A	250	VAL	2.1
1	A	76	SER	2.1
1	A	321	ASN	2.1
1	A	333	PRO	2.1
1	A	573	TYR	2.1
1	A	116	ALA	2.1
1	A	334	ALA	2.1
1	A	473	GLU	2.1
1	A	534	VAL	2.1
1	A	188	ALA	2.1
1	A	446	ASN	2.1
1	A	131	ASN	2.1
1	A	59	VAL	2.1
1	A	162	THR	2.0
1	A	294	LEU	2.0
1	A	579	ALA	2.0
1	A	499	PHE	2.0
1	A	215	ASP	2.0
1	A	106	VAL	2.0
1	A	267	PHE	2.0
1	A	479	LYS	2.0
1	A	476	THR	2.0
1	A	378	TYR	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	0.09	0.90	40,40,40,40	0
2	CA	A	586	1/1	0.38	0.71	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.