



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:10 AM GMT

PDB ID : 2ZTN
Title : Hepatitis E virus ORF2 (Genotype 3)
Authors : Yamashita, T.; Unno, H.; Mori, Y.; Li, T.C.; Takeda, N.; Matsuura, Y.
Deposited on : 2008-10-08
Resolution : 3.56 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

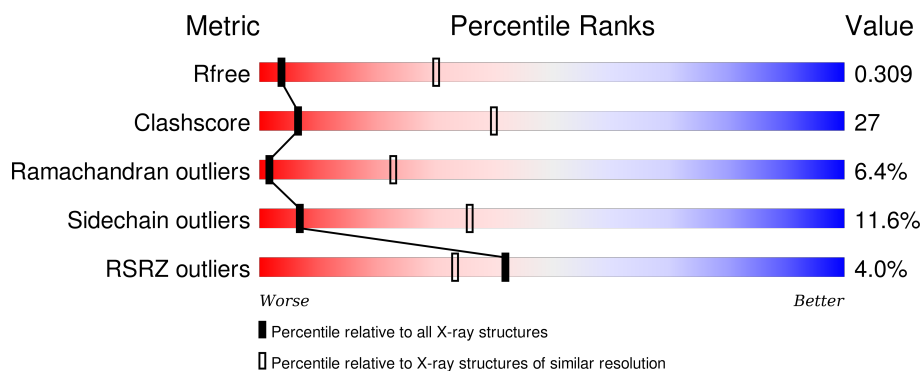
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 3.56 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))
R_{free}	91344	1240 (3.72-3.40)
Clashscore	102246	1057 (3.70-3.42)
Ramachandran outliers	100387	1017 (3.70-3.42)
Sidechain outliers	100360	1017 (3.70-3.42)
RSRZ outliers	91569	1247 (3.72-3.40)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	478	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3590 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

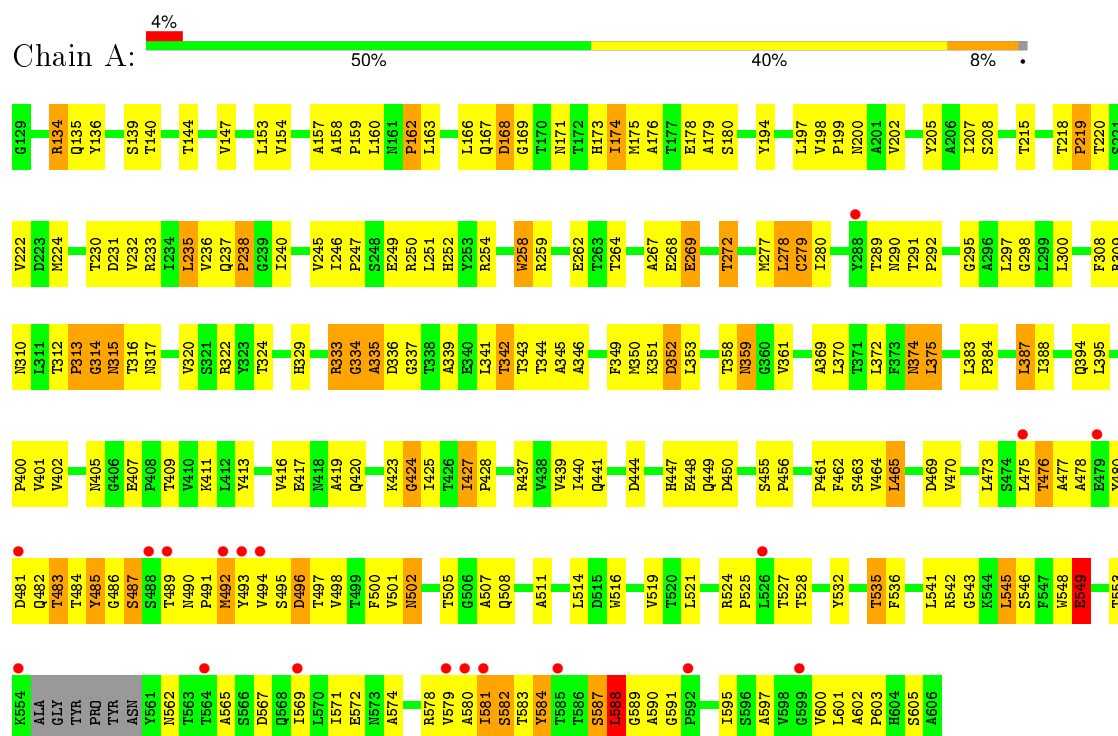
- Molecule 1 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	472	3590	2248	626	710	6	0	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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: Capsid protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	336.86Å 349.42Å 359.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.56 49.50 – 3.56	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-3.56) 98.8 (49.50-3.56)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 3.57Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.305 , 0.309 0.305 , 0.309	Depositor DCC
R_{free} test set	24621 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	105.6	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 61.2	EDS
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	0 of 498137 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	3590	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.50	0/3665	0.68	0/5015

There are no bond length outliers.

There are no bond angle outliers.

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	3590	0	3545	195	0
All	All	3590	0	3545	195	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 27.

All (195) 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:174:ILE:H	1:A:174:ILE:HD13	1.10	1.12
1:A:343:THR:HG22	1:A:345:ALA:H	1.16	1.05
1:A:543:GLY:H	1:A:565:ALA:HB1	1.28	0.95
1:A:174:ILE:N	1:A:174:ILE:HD13	1.88	0.88
1:A:154:VAL:HA	1:A:279:CYS:HB3	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ARG:HG2	1:A:136:TYR:CZ	2.12	0.84
1:A:475:LEU:HD12	1:A:595:ILE:HG23	1.60	0.84
1:A:322:ARG:HH11	1:A:441:GLN:HE21	1.24	0.83
1:A:174:ILE:H	1:A:174:ILE:CD1	1.81	0.83
1:A:237:GLN:HB3	1:A:238:PRO:HD2	1.65	0.78
1:A:375:LEU:HD12	1:A:375:LEU:H	1.48	0.77
1:A:197:LEU:HG	1:A:298:GLY:HA2	1.67	0.76
1:A:545:LEU:HD23	1:A:546:SER:H	1.51	0.75
1:A:478:ALA:HB3	1:A:495:SER:HA	1.68	0.75
1:A:353:LEU:HD23	1:A:448:GLU:HA	1.70	0.73
1:A:194:TYR:CZ	1:A:207:ILE:HD13	2.24	0.72
1:A:262:GLU:OE2	1:A:315:ASN:CG	2.27	0.72
1:A:258:TRP:O	1:A:259:ARG:HD3	1.90	0.72
1:A:478:ALA:HB2	1:A:496:ASP:H	1.56	0.71
1:A:163:LEU:HD21	1:A:316:THR:HG21	1.73	0.71
1:A:491:PRO:HG3	1:A:583:THR:O	1.91	0.70
1:A:208:SER:O	1:A:278:LEU:HA	1.92	0.70
1:A:153:LEU:HB2	1:A:280:ILE:HD11	1.74	0.70
1:A:489:THR:HG21	1:A:584:TYR:CD2	2.27	0.70
1:A:482:GLN:HG2	1:A:491:PRO:HA	1.73	0.69
1:A:486:GLY:HA3	1:A:490:ASN:HB2	1.76	0.68
1:A:329:HIS:HE1	1:A:343:THR:HG23	1.59	0.67
1:A:349:PHE:CZ	1:A:400:PRO:HD3	2.29	0.67
1:A:237:GLN:HB3	1:A:238:PRO:CD	2.25	0.67
1:A:542:ARG:HG3	1:A:602:ALA:HB2	1.77	0.66
1:A:455:SER:N	1:A:456:PRO:HD2	2.10	0.66
1:A:322:ARG:HG3	1:A:441:GLN:HG3	1.77	0.66
1:A:144:THR:HA	1:A:297:LEU:HD13	1.77	0.66
1:A:372:LEU:HB2	1:A:439:VAL:HB	1.78	0.65
1:A:289:THR:O	1:A:291:THR:HG23	1.96	0.65
1:A:383:LEU:HD23	1:A:384:PRO:HD2	1.78	0.65
1:A:329:HIS:CE1	1:A:343:THR:HG23	2.31	0.65
1:A:198:VAL:CG2	1:A:297:LEU:HA	2.26	0.65
1:A:316:THR:HG22	1:A:317:ASN:O	1.97	0.64
1:A:198:VAL:HG23	1:A:297:LEU:HA	1.79	0.64
1:A:516:TRP:HA	1:A:519:VAL:HG23	1.79	0.64
1:A:246:ILE:HD12	1:A:246:ILE:N	2.13	0.64
1:A:262:GLU:OE2	1:A:315:ASN:ND2	2.31	0.63
1:A:370:LEU:HD11	1:A:395:LEU:HD11	1.81	0.63
1:A:159:PRO:HB2	1:A:272:THR:OG1	1.99	0.62
1:A:262:GLU:OE2	1:A:315:ASN:OD1	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:GLY:O	1:A:335:ALA:C	2.38	0.61
1:A:322:ARG:HG3	1:A:441:GLN:CG	2.31	0.61
1:A:280:ILE:HD12	1:A:280:ILE:O	2.00	0.61
1:A:312:THR:O	1:A:314:GLY:N	2.34	0.61
1:A:542:ARG:HH21	1:A:603:PRO:CD	2.14	0.60
1:A:342:THR:HG23	1:A:409:THR:OG1	2.01	0.60
1:A:199:PRO:O	1:A:202:VAL:HG23	2.01	0.60
1:A:136:TYR:CD1	1:A:175:MET:HE2	2.36	0.60
1:A:375:LEU:HD12	1:A:375:LEU:N	2.15	0.60
1:A:180:SER:O	1:A:314:GLY:HA2	2.01	0.60
1:A:322:ARG:NH1	1:A:441:GLN:HE21	1.98	0.60
1:A:545:LEU:HD23	1:A:546:SER:N	2.17	0.59
1:A:247:PRO:HG2	1:A:250:ARG:HG2	1.83	0.59
1:A:528:THR:HG23	1:A:535:THR:HG22	1.85	0.59
1:A:134:ARG:HG3	1:A:135:GLN:N	2.16	0.58
1:A:343:THR:HG22	1:A:345:ALA:N	2.01	0.58
1:A:247:PRO:HG2	1:A:250:ARG:CG	2.33	0.58
1:A:562:ASN:ND2	1:A:584:TYR:OH	2.38	0.57
1:A:174:ILE:O	1:A:178:GLU:HG3	2.05	0.57
1:A:494:VAL:CG1	1:A:578:ARG:HD3	2.34	0.57
1:A:230:THR:HG22	1:A:231:ASP:N	2.18	0.57
1:A:494:VAL:HG13	1:A:578:ARG:HD3	1.87	0.57
1:A:346:ALA:O	1:A:350:MET:HG2	2.05	0.56
1:A:462:PHE:CZ	1:A:500:PHE:HB3	2.40	0.56
1:A:480:TYR:CD2	1:A:493:TYR:HB3	2.41	0.56
1:A:584:TYR:H	1:A:584:TYR:HD1	1.51	0.56
1:A:489:THR:HG23	1:A:584:TYR:HA	1.86	0.56
1:A:339:ALA:HA	1:A:427:ILE:HD11	1.87	0.56
1:A:401:VAL:HG21	1:A:411:LYS:HB2	1.88	0.56
1:A:350:MET:HE1	1:A:409:THR:O	2.06	0.55
1:A:498:VAL:H	1:A:511:ALA:HB2	1.72	0.55
1:A:254:ARG:HB3	1:A:259:ARG:NH2	2.21	0.55
1:A:162:PRO:HA	1:A:175:MET:SD	2.48	0.54
1:A:491:PRO:HG3	1:A:583:THR:C	2.28	0.54
1:A:167:GLN:HG2	1:A:171:ASN:ND2	2.23	0.54
1:A:501:VAL:HG22	1:A:508:GLN:HG2	1.89	0.53
1:A:492:MET:HG3	1:A:580:ALA:CB	2.39	0.53
1:A:483:THR:HG21	1:A:532:TYR:HD1	1.74	0.53
1:A:423:LYS:O	1:A:424:GLY:O	2.27	0.53
1:A:587:SER:O	1:A:589:GLY:N	2.42	0.52
1:A:246:ILE:HG21	1:A:251:LEU:HD21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:GLY:N	1:A:565:ALA:HB1	2.11	0.52
1:A:374:ASN:HB2	1:A:437:ARG:HB3	1.89	0.52
1:A:291:THR:HB	1:A:292:PRO:HD2	1.92	0.52
1:A:465:LEU:O	1:A:521:LEU:HA	2.09	0.52
1:A:475:LEU:HD23	1:A:498:VAL:CG1	2.40	0.52
1:A:524:ARG:HG2	1:A:525:PRO:HD2	1.91	0.52
1:A:545:LEU:HD13	1:A:581:ILE:HG23	1.92	0.51
1:A:545:LEU:HD21	1:A:597:ALA:HB1	1.91	0.51
1:A:473:LEU:HD22	1:A:500:PHE:CD2	2.45	0.51
1:A:416:VAL:O	1:A:420:GLN:HG3	2.10	0.51
1:A:339:ALA:CB	1:A:427:ILE:HD11	2.41	0.51
1:A:259:ARG:NH1	1:A:272:THR:O	2.44	0.51
1:A:486:GLY:CA	1:A:490:ASN:HB2	2.40	0.51
1:A:486:GLY:HA2	1:A:532:TYR:OH	2.10	0.51
1:A:167:GLN:HG2	1:A:171:ASN:CG	2.31	0.51
1:A:571:ILE:HD12	1:A:571:ILE:N	2.26	0.50
1:A:465:LEU:HD22	1:A:601:LEU:HD11	1.93	0.50
1:A:505:THR:HG22	1:A:507:ALA:H	1.75	0.50
1:A:502:ASN:C	1:A:502:ASN:HD22	2.14	0.50
1:A:486:GLY:HA3	1:A:490:ASN:CB	2.42	0.50
1:A:478:ALA:HB2	1:A:496:ASP:N	2.24	0.50
1:A:268:GLU:HG3	1:A:416:VAL:HG21	1.94	0.50
1:A:427:ILE:HG22	1:A:428:PRO:HD2	1.94	0.50
1:A:481:ASP:O	1:A:482:GLN:HB2	2.12	0.49
1:A:343:THR:HG22	1:A:344:THR:N	2.27	0.49
1:A:536:PHE:CE2	1:A:572:GLU:HB3	2.47	0.49
1:A:309:ARG:O	1:A:310:ASN:HB2	2.11	0.49
1:A:264:THR:HG23	1:A:444:ASP:OD2	2.12	0.49
1:A:475:LEU:HD23	1:A:498:VAL:HG13	1.95	0.49
1:A:316:THR:HG22	1:A:317:ASN:N	2.28	0.48
1:A:333:ARG:HB3	1:A:427:ILE:HD12	1.95	0.48
1:A:489:THR:HG21	1:A:584:TYR:CG	2.48	0.48
1:A:387:LEU:CD2	1:A:425:ILE:HG21	2.43	0.48
1:A:205:TYR:HE1	1:A:207:ILE:HD11	1.77	0.48
1:A:267:ALA:HB1	1:A:269:GLU:OE2	2.14	0.48
1:A:405:ASN:HD22	1:A:407:GLU:HB2	1.79	0.47
1:A:370:LEU:HB3	1:A:441:GLN:HB2	1.95	0.47
1:A:246:ILE:N	1:A:246:ILE:CD1	2.77	0.47
1:A:173:HIS:CE1	1:A:176:ALA:H	2.33	0.47
1:A:179:ALA:HB2	1:A:308:PHE:CZ	2.50	0.47
1:A:218:THR:HG23	1:A:395:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:VAL:HG11	1:A:277:MET:HE1	1.97	0.47
1:A:268:GLU:O	1:A:272:THR:HB	2.15	0.47
1:A:297:LEU:HD12	1:A:297:LEU:N	2.30	0.47
1:A:198:VAL:HG11	1:A:202:VAL:HB	1.97	0.47
1:A:324:THR:HG23	1:A:439:VAL:HG22	1.97	0.46
1:A:157:ALA:O	1:A:158:ALA:HB2	2.15	0.46
1:A:207:ILE:O	1:A:235:LEU:HD23	2.16	0.46
1:A:553:THR:HG21	1:A:588:LEU:HG	1.98	0.46
1:A:542:ARG:CG	1:A:602:ALA:HB2	2.45	0.46
1:A:492:MET:HG3	1:A:580:ALA:HB3	1.98	0.46
1:A:341:LEU:O	1:A:409:THR:HA	2.16	0.45
1:A:571:ILE:HA	1:A:578:ARG:O	2.16	0.45
1:A:447:HIS:HB3	1:A:450:ASP:HB2	1.99	0.45
1:A:322:ARG:HH11	1:A:441:GLN:NE2	2.02	0.45
1:A:252:HIS:ND1	1:A:252:HIS:N	2.65	0.45
1:A:343:THR:CG2	1:A:344:THR:N	2.79	0.45
1:A:278:LEU:O	1:A:278:LEU:HD23	2.16	0.44
1:A:405:ASN:ND2	1:A:407:GLU:HB2	2.31	0.44
1:A:447:HIS:HE1	1:A:449:GLN:HG2	1.82	0.44
1:A:542:ARG:HH21	1:A:603:PRO:HD3	1.83	0.44
1:A:339:ALA:CA	1:A:427:ILE:HD11	2.48	0.44
1:A:484:THR:O	1:A:485:TYR:HB3	2.18	0.44
1:A:581:ILE:HG22	1:A:582:SER:H	1.82	0.44
1:A:147:VAL:HG21	1:A:374:ASN:HB3	2.00	0.44
1:A:475:LEU:HD12	1:A:595:ILE:CG2	2.39	0.43
1:A:387:LEU:HD21	1:A:425:ILE:HG21	1.98	0.43
1:A:140:THR:HG22	1:A:166:LEU:HA	2.00	0.43
1:A:375:LEU:N	1:A:375:LEU:CD1	2.80	0.43
1:A:548:TRP:CE3	1:A:597:ALA:HA	2.53	0.43
1:A:316:THR:CG2	1:A:317:ASN:N	2.81	0.43
1:A:222:VAL:CG1	1:A:277:MET:HE1	2.49	0.43
1:A:542:ARG:HH21	1:A:603:PRO:CG	2.32	0.43
1:A:372:LEU:HA	1:A:394:GLN:O	2.19	0.43
1:A:470:VAL:HG22	1:A:600:VAL:HG22	2.00	0.43
1:A:160:LEU:HA	1:A:160:LEU:HD23	1.86	0.43
1:A:548:TRP:H	1:A:595:ILE:HG13	1.84	0.43
1:A:447:HIS:CE1	1:A:449:GLN:HG2	2.54	0.42
1:A:475:LEU:O	1:A:476:THR:C	2.58	0.42
1:A:369:ALA:HB1	1:A:441:GLN:O	2.19	0.42
1:A:315:ASN:ND2	1:A:315:ASN:O	2.52	0.42
1:A:461:PRO:HG2	1:A:464:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:TYR:CD2	1:A:419:ALA:HA	2.54	0.42
1:A:322:ARG:HA	1:A:440:ILE:O	2.18	0.42
1:A:473:LEU:HD11	1:A:569:ILE:HD13	2.00	0.42
1:A:579:VAL:HG12	1:A:580:ALA:H	1.83	0.42
1:A:579:VAL:HG12	1:A:580:ALA:N	2.35	0.42
1:A:548:TRP:CZ3	1:A:597:ALA:HA	2.54	0.42
1:A:455:SER:N	1:A:456:PRO:CD	2.80	0.42
1:A:140:THR:HA	1:A:166:LEU:HB3	2.01	0.42
1:A:463:SER:OG	1:A:514:LEU:HD11	2.19	0.42
1:A:352:ASP:OD1	1:A:352:ASP:C	2.58	0.42
1:A:492:MET:HG3	1:A:580:ALA:HB1	2.01	0.42
1:A:480:TYR:O	1:A:482:GLN:NE2	2.53	0.42
1:A:542:ARG:HE	1:A:603:PRO:HD3	1.85	0.42
1:A:218:THR:O	1:A:219:PRO:C	2.55	0.41
1:A:198:VAL:HG13	1:A:199:PRO:HD2	2.01	0.41
1:A:198:VAL:CG1	1:A:202:VAL:HB	2.50	0.41
1:A:333:ARG:NH1	1:A:337:GLY:HA2	2.35	0.41
1:A:168:ASP:O	1:A:322:ARG:O	2.37	0.41
1:A:486:GLY:O	1:A:487:SER:O	2.39	0.41
1:A:516:TRP:HA	1:A:519:VAL:CG2	2.48	0.41
1:A:572:GLU:OE1	1:A:574:ALA:HB3	2.20	0.41
1:A:144:THR:HA	1:A:297:LEU:CD1	2.48	0.41
1:A:351:LYS:O	1:A:448:GLU:HG3	2.21	0.41
1:A:541:LEU:HD11	1:A:569:ILE:CD1	2.51	0.40
1:A:548:TRP:HB3	1:A:549:GLU:H	1.77	0.40
1:A:588:LEU:HA	1:A:588:LEU:HD13	1.91	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	468/478 (98%)	383 (82%)	55 (12%)	30 (6%)	2 23

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	313	PRO
1	A	335	ALA
1	A	358	THR
1	A	476	THR
1	A	477	ALA
1	A	487	SER
1	A	549	GLU
1	A	588	LEU
1	A	605	SER
1	A	220	THR
1	A	224	MET
1	A	314	GLY
1	A	359	ASN
1	A	424	GLY
1	A	587	SER
1	A	590	ALA
1	A	200	ASN
1	A	483	THR
1	A	169	GLY
1	A	581	ILE
1	A	582	SER
1	A	591	GLY
1	A	485	TYR
1	A	232	VAL
1	A	240	ILE
1	A	334	GLY
1	A	219	PRO
1	A	361	VAL
1	A	295	GLY
1	A	162	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	395/399 (99%)	349 (88%)	46 (12%)	7 36

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	ARG
1	A	139	SER
1	A	168	ASP
1	A	174	ILE
1	A	215	THR
1	A	233	ARG
1	A	235	LEU
1	A	236	VAL
1	A	238	PRO
1	A	245	VAL
1	A	249	GLU
1	A	258	TRP
1	A	269	GLU
1	A	272	THR
1	A	278	LEU
1	A	279	CYS
1	A	290	ASN
1	A	300	LEU
1	A	313	PRO
1	A	315	ASN
1	A	320	VAL
1	A	333	ARG
1	A	336	ASP
1	A	342	THR
1	A	352	ASP
1	A	359	ASN
1	A	374	ASN
1	A	375	LEU
1	A	387	LEU
1	A	388	ILE
1	A	402	VAL
1	A	417	GLU
1	A	427	ILE
1	A	465	LEU
1	A	469	ASP
1	A	492	MET

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Mol	Chain	Res	Type
1	A	496	ASP
1	A	497	THR
1	A	502	ASN
1	A	527	THR
1	A	535	THR
1	A	545	LEU
1	A	549	GLU
1	A	567	ASP
1	A	584	TYR
1	A	588	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	171	ASN
1	A	315	ASN
1	A	329	HIS
1	A	441	GLN
1	A	482	GLN
1	A	490	ASN
1	A	502	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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, 95th 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	472/478 (98%)	0.24	19 (4%) 42 33	74, 108, 172, 187	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	493	TYR	3.7
1	A	492	MET	3.6
1	A	585	THR	3.4
1	A	494	VAL	3.4
1	A	592	PRO	3.3
1	A	481	ASP	3.3
1	A	580	ALA	2.5
1	A	579	VAL	2.5
1	A	564	THR	2.5
1	A	488	SER	2.4
1	A	599	GLY	2.3
1	A	489	THR	2.3
1	A	526	LEU	2.2
1	A	569	ILE	2.2
1	A	554	LYS	2.2
1	A	479	GLU	2.2
1	A	581	ILE	2.1
1	A	288	TYR	2.1
1	A	475	LEU	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 [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.