Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:12 AM GMT

PDB ID	:	2ZZQ
Title	:	Crystal structure analysis of the HEV capsid protein, PORF2
Authors	:	Miyazaki, N.; Xing, L.; Wang, C.-Y.; Li, T.-C.; Takeda, N.; Higashiura, A.; Nakagawa, A.; Tsukihara, T.; Miyamura, T.; Cheng, R.H.
Deposited on	:	2009-02-23
Resolution	:	3.81 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 ①) were used in the production of this report:

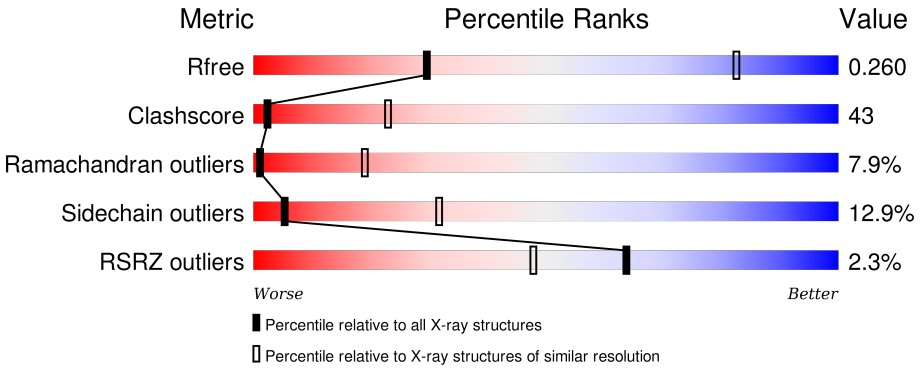
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.81 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	1324 (4.14-3.50)
Clashscore	102246	1028 (4.12-3.52)
Ramachandran outliers	100387	1404 (4.14-3.50)
Sidechain outliers	100360	1399 (4.14-3.50)
RSRZ outliers	91569	1332 (4.14-3.50)

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 <=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	552	2% 36% 41% 10% 13%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3658 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 Protein ORF3, Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	483	3658	2292	636	725	5	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

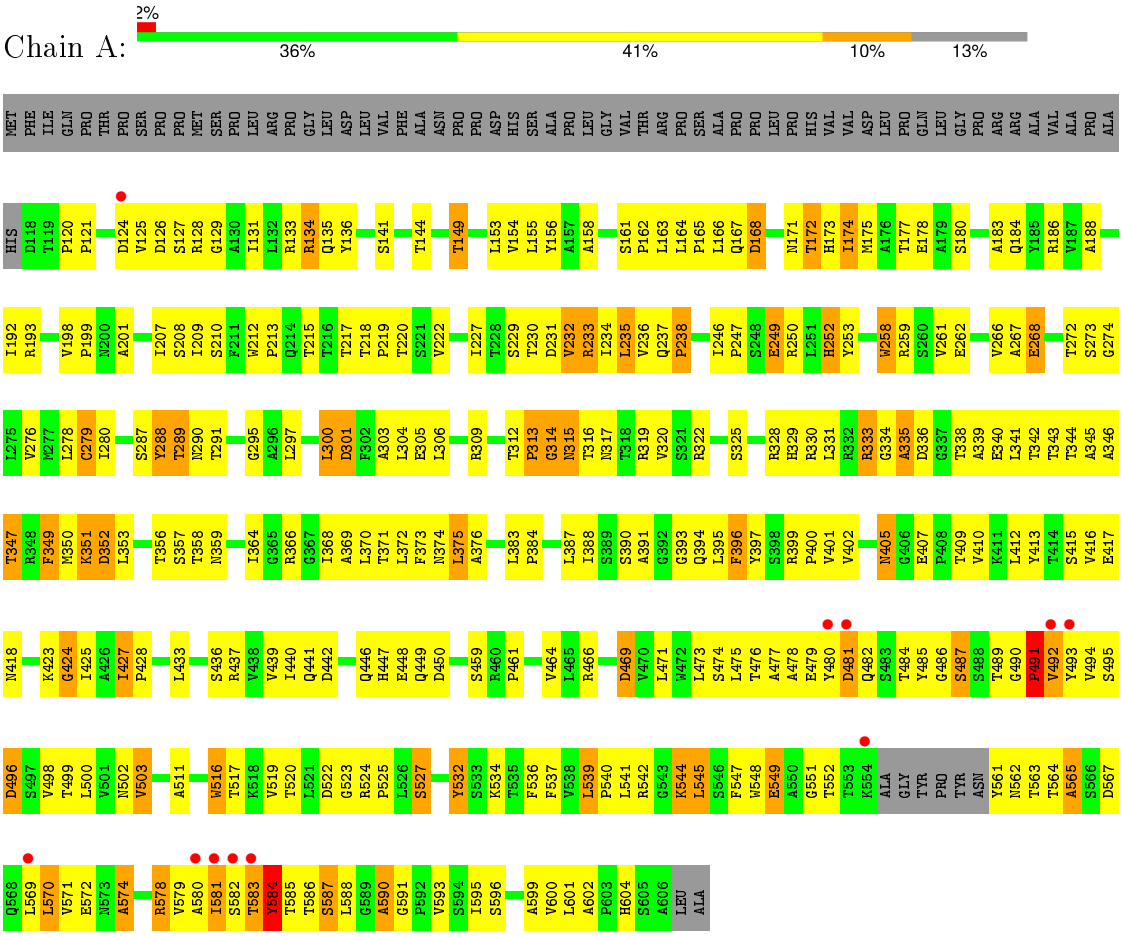
Chain	Residue	Modelled	Actual	Comment	Reference
A	57	MET	-	INITIATING METHIONINE	UNP P69616
A	284	PRO	LEU	CONFLICT	UNP P29326

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 (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: Protein ORF3, Capsid protein

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	337.00Å 347.00Å 354.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.81 69.37 – 3.81	Depositor EDS
% Data completeness (in resolution range)	68.8 (20.00-3.81) 69.1 (69.37-3.81)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 3.77Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.242 , 0.245 0.262 , 0.260	Depositor DCC
R_{free} test set	13812 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	131.8	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 52.1	EDS
Estimated twinning fraction	0.034 for -h,l,k 0.036 for -l,-k,-h 0.035 for k,h,-l 0.034 for k,l,h 0.034 for l,h,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Outliers	0 of 277894 reflections	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	3658	wwPDB-VP
Average B, all atoms (Å^2)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.51	0/3735	0.79	0/5114

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

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	3658	0	3615	312	0
All	All	3658	0	3615	312	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 43.

All (312) 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:343:THR:HG22	1:A:345:ALA:H	1.12	1.06
1:A:549:GLU:HG3	1:A:588:LEU:HD11	1.36	1.06
1:A:478:ALA:HB2	1:A:496:ASP:H	1.13	1.05
1:A:478:ALA:HB3	1:A:495:SER:HA	1.42	0.98
1:A:272:THR:HG22	1:A:273:SER:H	1.27	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:LEU:HD22	1:A:569:LEU:HG	1.49	0.95
1:A:370:LEU:HD11	1:A:395:LEU:HD11	1.47	0.94
1:A:485:TYR:HA	1:A:490:GLY:O	1.69	0.92
1:A:218:THR:HG23	1:A:395:LEU:HD23	1.52	0.92
1:A:478:ALA:HB2	1:A:496:ASP:N	1.85	0.90
1:A:474:SER:HB2	1:A:499:THR:HB	1.55	0.88
1:A:473:LEU:HD22	1:A:500:LEU:HD22	1.57	0.86
1:A:549:GLU:CG	1:A:588:LEU:HD11	2.05	0.85
1:A:180:SER:O	1:A:314:GLY:HA2	1.76	0.85
1:A:209:ILE:HG12	1:A:278:LEU:HD13	1.59	0.85
1:A:534:LYS:HB2	1:A:536:PHE:HE1	1.42	0.84
1:A:482:GLN:HE22	1:A:586:THR:HG23	1.41	0.84
1:A:201:ALA:HB1	1:A:288:TYR:HE2	1.43	0.84
1:A:158:ALA:HB1	1:A:164:LEU:HD11	1.58	0.83
1:A:492:VAL:HA	1:A:581:ILE:O	1.79	0.81
1:A:478:ALA:CB	1:A:495:SER:HA	2.12	0.79
1:A:375:LEU:HD12	1:A:375:LEU:H	1.47	0.79
1:A:541:LEU:HD21	1:A:599:ALA:HB1	1.63	0.79
1:A:339:ALA:CA	1:A:427:ILE:HD11	2.13	0.79
1:A:475:LEU:HD13	1:A:495:SER:HB3	1.64	0.78
1:A:339:ALA:HA	1:A:427:ILE:HD11	1.66	0.78
1:A:272:THR:HG22	1:A:273:SER:N	1.97	0.76
1:A:201:ALA:HB1	1:A:288:TYR:CE2	2.20	0.76
1:A:588:LEU:HD13	1:A:593:VAL:HG11	1.69	0.75
1:A:482:GLN:NE2	1:A:586:THR:HG23	2.03	0.73
1:A:548:TRP:HB2	1:A:596:SER:O	1.87	0.73
1:A:188:ALA:HB3	1:A:305:GLU:HB3	1.71	0.73
1:A:349:PHE:CZ	1:A:400:PRO:HD3	2.24	0.72
1:A:584:TYR:N	1:A:584:TYR:CD1	2.57	0.72
1:A:447:HIS:HB3	1:A:450:ASP:HB2	1.70	0.72
1:A:186:ARG:HB2	1:A:258:TRP:CD1	2.23	0.72
1:A:134:ARG:HG3	1:A:135:GLN:N	2.03	0.72
1:A:475:LEU:HD23	1:A:498:VAL:HG13	1.71	0.72
1:A:516:TRP:HA	1:A:519:VAL:HG23	1.70	0.71
1:A:473:LEU:HA	1:A:499:THR:O	1.90	0.70
1:A:322:ARG:NH1	1:A:441:GLN:HE21	1.89	0.70
1:A:539:LEU:HD13	1:A:601:LEU:HD21	1.74	0.70
1:A:322:ARG:HH11	1:A:441:GLN:HE21	1.40	0.70
1:A:201:ALA:CB	1:A:288:TYR:HE2	2.04	0.70
1:A:201:ALA:CB	1:A:288:TYR:CE2	2.75	0.70
1:A:498:VAL:HB	1:A:511:ALA:HB2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:PHE:CE2	1:A:572:GLU:HB3	2.27	0.69
1:A:345:ALA:HB1	1:A:440:ILE:HG12	1.72	0.69
1:A:489:THR:O	1:A:491:PRO:HD3	1.92	0.69
1:A:333:ARG:HB2	1:A:427:ILE:HD12	1.74	0.69
1:A:167:GLN:HG2	1:A:171:ASN:ND2	2.08	0.69
1:A:516:TRP:HA	1:A:519:VAL:CG2	2.23	0.68
1:A:588:LEU:HD22	1:A:593:VAL:HG21	1.76	0.68
1:A:583:THR:HG22	1:A:583:THR:O	1.92	0.68
1:A:549:GLU:OE2	1:A:588:LEU:HD21	1.95	0.67
1:A:537:PHE:N	1:A:571:VAL:O	2.26	0.67
1:A:372:LEU:HB2	1:A:439:VAL:HB	1.75	0.67
1:A:250:ARG:HH11	1:A:250:ARG:HG2	1.60	0.67
1:A:342:THR:HG22	1:A:409:THR:OG1	1.95	0.67
1:A:548:TRP:O	1:A:595:ILE:HG13	1.94	0.67
1:A:491:PRO:HG3	1:A:583:THR:C	2.15	0.67
1:A:370:LEU:HB3	1:A:441:GLN:HB2	1.75	0.67
1:A:164:LEU:HD23	1:A:166:LEU:HD21	1.77	0.67
1:A:552:THR:O	1:A:552:THR:HG22	1.95	0.66
1:A:289:THR:O	1:A:291:THR:HG23	1.95	0.66
1:A:586:THR:O	1:A:586:THR:HG22	1.95	0.66
1:A:570:LEU:HB2	1:A:580:ALA:HB3	1.77	0.66
1:A:341:LEU:C	1:A:409:THR:HG23	2.16	0.66
1:A:541:LEU:HD11	1:A:599:ALA:HB1	1.76	0.65
1:A:258:TRP:O	1:A:259:ARG:HD3	1.96	0.65
1:A:272:THR:HG22	1:A:274:GLY:H	1.59	0.65
1:A:368:ILE:HD12	1:A:368:ILE:N	2.12	0.65
1:A:544:LYS:N	1:A:544:LYS:HD2	2.11	0.65
1:A:162:PRO:HA	1:A:175:MET:SD	2.37	0.65
1:A:272:THR:CG2	1:A:273:SER:H	2.07	0.65
1:A:198:VAL:CG2	1:A:297:LEU:HA	2.27	0.64
1:A:484:THR:HG23	1:A:532:TYR:CD1	2.33	0.63
1:A:192:ILE:CD1	1:A:276:VAL:HG11	2.28	0.63
1:A:373:PHE:O	1:A:394:GLN:HG2	1.98	0.63
1:A:193:ARG:HG2	1:A:301:ASP:HB3	1.81	0.63
1:A:230:THR:HG22	1:A:231:ASP:N	2.15	0.62
1:A:312:THR:O	1:A:314:GLY:N	2.32	0.61
1:A:541:LEU:HB3	1:A:567:ASP:O	1.99	0.61
1:A:331:LEU:HB2	1:A:433:LEU:HD11	1.83	0.61
1:A:478:ALA:CB	1:A:496:ASP:H	2.02	0.61
1:A:478:ALA:CB	1:A:496:ASP:N	2.63	0.61
1:A:480:TYR:HB3	1:A:493:TYR:HD2	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:PRO:HA	1:A:410:VAL:HG12	1.84	0.60
1:A:184:GLN:HB2	1:A:309:ARG:HG3	1.82	0.60
1:A:343:THR:HG22	1:A:345:ALA:N	1.98	0.60
1:A:207:ILE:HG22	1:A:278:LEU:HD11	1.83	0.60
1:A:165:PRO:HB3	1:A:320:VAL:CG1	2.32	0.60
1:A:329:HIS:O	1:A:433:LEU:HB2	2.02	0.60
1:A:480:TYR:HB3	1:A:493:TYR:CD2	2.37	0.60
1:A:364:ILE:N	1:A:364:ILE:HD12	2.17	0.59
1:A:350:MET:HE1	1:A:409:THR:O	2.02	0.59
1:A:198:VAL:HG23	1:A:297:LEU:O	2.02	0.59
1:A:489:THR:HG1	1:A:584:TYR:HE2	1.51	0.59
1:A:547:PHE:CZ	1:A:583:THR:HB	2.37	0.59
1:A:218:THR:CG2	1:A:395:LEU:HD23	2.28	0.59
1:A:333:ARG:HG3	1:A:333:ARG:O	2.01	0.59
1:A:423:LYS:O	1:A:424:GLY:O	2.22	0.58
1:A:351:LYS:HB3	1:A:448:GLU:OE2	2.03	0.58
1:A:585:THR:HG22	1:A:586:THR:H	1.68	0.58
1:A:405:ASN:C	1:A:407:GLU:H	2.07	0.58
1:A:266:VAL:HG12	1:A:267:ALA:H	1.67	0.57
1:A:480:TYR:CB	1:A:493:TYR:HD2	2.18	0.57
1:A:583:THR:O	1:A:585:THR:N	2.37	0.57
1:A:183:ALA:O	1:A:261:VAL:HG23	2.04	0.57
1:A:168:ASP:O	1:A:322:ARG:O	2.21	0.57
1:A:373:PHE:HB2	1:A:394:GLN:HA	1.87	0.57
1:A:329:HIS:CE1	1:A:343:THR:HG23	2.41	0.56
1:A:477:ALA:HA	1:A:593:VAL:O	2.05	0.56
1:A:186:ARG:HB2	1:A:258:TRP:NE1	2.19	0.56
1:A:481:ASP:O	1:A:482:GLN:HB2	2.06	0.56
1:A:207:ILE:CG2	1:A:278:LEU:HD11	2.35	0.56
1:A:439:VAL:O	1:A:440:ILE:HD13	2.06	0.56
1:A:259:ARG:NH1	1:A:273:SER:HA	2.20	0.56
1:A:163:LEU:HD21	1:A:316:THR:HG21	1.88	0.56
1:A:153:LEU:HD22	1:A:374:ASN:ND2	2.21	0.56
1:A:144:THR:O	1:A:437:ARG:NH1	2.39	0.55
1:A:297:LEU:HD12	1:A:297:LEU:N	2.20	0.55
1:A:563:THR:O	1:A:565:ALA:N	2.39	0.55
1:A:585:THR:HG22	1:A:587:SER:H	1.71	0.55
1:A:572:GLU:CD	1:A:574:ALA:HB3	2.27	0.55
1:A:193:ARG:CG	1:A:301:ASP:HB3	2.36	0.55
1:A:230:THR:HG22	1:A:231:ASP:H	1.72	0.54
1:A:548:TRP:HB2	1:A:596:SER:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ALA:CB	1:A:427:ILE:HD11	2.38	0.54
1:A:329:HIS:HE1	1:A:343:THR:HG23	1.73	0.54
1:A:356:THR:O	1:A:356:THR:HG22	2.07	0.54
1:A:184:GLN:HB2	1:A:309:ARG:HB2	1.89	0.53
1:A:415:SER:OG	1:A:416:VAL:N	2.42	0.53
1:A:136:TYR:CD1	1:A:175:MET:HE2	2.43	0.53
1:A:164:LEU:CD2	1:A:166:LEU:HD21	2.38	0.53
1:A:534:LYS:CB	1:A:536:PHE:HE1	2.18	0.53
1:A:370:LEU:HD13	1:A:397:TYR:CE2	2.44	0.53
1:A:415:SER:HB3	1:A:418:ASN:HD22	1.73	0.53
1:A:314:GLY:C	1:A:316:THR:H	2.12	0.53
1:A:249:GLU:O	1:A:249:GLU:HG3	2.07	0.52
1:A:549:GLU:C	1:A:551:GLY:N	2.62	0.52
1:A:541:LEU:HD21	1:A:599:ALA:CB	2.36	0.52
1:A:165:PRO:HB3	1:A:320:VAL:HG11	1.92	0.52
1:A:222:VAL:HG12	1:A:222:VAL:O	2.10	0.52
1:A:466:ARG:O	1:A:469:ASP:HB2	2.09	0.52
1:A:491:PRO:HD2	1:A:582:SER:CB	2.40	0.51
1:A:272:THR:HG22	1:A:274:GLY:N	2.24	0.51
1:A:384:PRO:HD2	1:A:387:LEU:HD12	1.91	0.51
1:A:192:ILE:HD12	1:A:276:VAL:HG11	1.91	0.51
1:A:266:VAL:HG12	1:A:267:ALA:N	2.25	0.51
1:A:375:LEU:N	1:A:375:LEU:HD12	2.20	0.51
1:A:590:ALA:HB3	1:A:593:VAL:HG21	1.92	0.51
1:A:237:GLN:HB3	1:A:238:PRO:HD2	1.93	0.51
1:A:208:SER:O	1:A:278:LEU:HD12	2.10	0.51
1:A:172:THR:HG23	1:A:173:HIS:N	2.25	0.51
1:A:303:ALA:C	1:A:304:LEU:HD23	2.31	0.51
1:A:396:PHE:CD1	1:A:396:PHE:N	2.79	0.51
1:A:325:SER:OG	1:A:344:THR:HB	2.11	0.50
1:A:339:ALA:HB2	1:A:427:ILE:HD11	1.93	0.50
1:A:154:VAL:HA	1:A:279:CYS:HB3	1.92	0.50
1:A:346:ALA:O	1:A:347:THR:C	2.50	0.50
1:A:233:ARG:N	1:A:233:ARG:HD3	2.26	0.50
1:A:156:TYR:CE2	1:A:158:ALA:HB2	2.46	0.50
1:A:447:HIS:HD1	1:A:448:GLU:N	2.09	0.50
1:A:484:THR:HG23	1:A:532:TYR:CE1	2.47	0.50
1:A:233:ARG:H	1:A:233:ARG:HD3	1.77	0.50
1:A:412:LEU:HB3	1:A:425:ILE:HD12	1.94	0.49
1:A:357:SER:O	1:A:358:THR:C	2.51	0.49
1:A:491:PRO:HD2	1:A:582:SER:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:GLU:C	1:A:481:ASP:H	2.16	0.49
1:A:153:LEU:HD22	1:A:374:ASN:HD22	1.78	0.49
1:A:489:THR:HG23	1:A:584:TYR:CE2	2.47	0.49
1:A:198:VAL:HG22	1:A:297:LEU:HA	1.93	0.49
1:A:461:PRO:HG2	1:A:464:VAL:HG23	1.94	0.49
1:A:350:MET:HE3	1:A:409:THR:H	1.78	0.49
1:A:320:VAL:HG13	1:A:442:ASP:HB2	1.94	0.49
1:A:491:PRO:HG3	1:A:583:THR:N	2.26	0.49
1:A:588:LEU:CD1	1:A:593:VAL:HG11	2.42	0.49
1:A:415:SER:HB3	1:A:418:ASN:ND2	2.27	0.49
1:A:485:TYR:O	1:A:487:SER:N	2.45	0.49
1:A:350:MET:CE	1:A:409:THR:H	2.26	0.48
1:A:338:THR:HA	1:A:425:ILE:O	2.13	0.48
1:A:155:LEU:HD11	1:A:280:ILE:HG12	1.95	0.48
1:A:259:ARG:NH1	1:A:272:THR:O	2.46	0.48
1:A:161:SER:O	1:A:164:LEU:HB2	2.13	0.48
1:A:390:SER:O	1:A:391:ALA:HB3	2.12	0.48
1:A:471:LEU:HD11	1:A:601:LEU:HD11	1.94	0.48
1:A:371:THR:N	1:A:396:PHE:O	2.46	0.48
1:A:586:THR:C	1:A:588:LEU:H	2.16	0.48
1:A:590:ALA:HB3	1:A:593:VAL:CG2	2.44	0.48
1:A:541:LEU:CD2	1:A:599:ALA:HB1	2.40	0.48
1:A:316:THR:HG22	1:A:317:ASN:O	2.13	0.48
1:A:352:ASP:HB2	1:A:446:GLN:O	2.13	0.48
1:A:544:LYS:H	1:A:544:LYS:HD2	1.77	0.48
1:A:427:ILE:HG22	1:A:428:PRO:HD2	1.96	0.48
1:A:401:VAL:HG12	1:A:402:VAL:N	2.28	0.48
1:A:447:HIS:ND1	1:A:448:GLU:N	2.60	0.48
1:A:548:TRP:H	1:A:595:ILE:CG1	2.27	0.47
1:A:288:TYR:N	1:A:288:TYR:HD2	2.12	0.47
1:A:136:TYR:CE2	1:A:175:MET:HA	2.49	0.47
1:A:288:TYR:CD2	1:A:288:TYR:N	2.82	0.47
1:A:473:LEU:HD22	1:A:500:LEU:CD2	2.37	0.47
1:A:542:ARG:CB	1:A:602:ALA:HB2	2.43	0.47
1:A:583:THR:CG2	1:A:583:THR:O	2.61	0.47
1:A:498:VAL:HG21	1:A:579:VAL:CG2	2.45	0.47
1:A:207:ILE:O	1:A:235:LEU:HD23	2.15	0.47
1:A:174:ILE:H	1:A:174:ILE:HG13	1.45	0.47
1:A:393:GLY:O	1:A:394:GLN:HG3	2.13	0.47
1:A:131:ILE:HG22	1:A:131:ILE:O	2.15	0.47
1:A:541:LEU:HD22	1:A:569:LEU:CG	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:THR:CG2	1:A:173:HIS:N	2.76	0.46
1:A:208:SER:O	1:A:278:LEU:HA	2.15	0.46
1:A:548:TRP:CB	1:A:596:SER:H	2.28	0.46
1:A:405:ASN:O	1:A:407:GLU:N	2.46	0.46
1:A:184:GLN:HB2	1:A:309:ARG:CG	2.45	0.46
1:A:345:ALA:CB	1:A:440:ILE:HG12	2.42	0.46
1:A:149:THR:O	1:A:376:ALA:HA	2.15	0.46
1:A:544:LYS:O	1:A:545:LEU:O	2.34	0.46
1:A:542:ARG:HB2	1:A:602:ALA:HB2	1.98	0.46
1:A:192:ILE:HD13	1:A:276:VAL:HG11	1.97	0.45
1:A:120:PRO:HA	1:A:121:PRO:HD3	1.70	0.45
1:A:250:ARG:HG2	1:A:250:ARG:NH1	2.30	0.45
1:A:262:GLU:OE2	1:A:315:ASN:CG	2.54	0.45
1:A:343:THR:CG2	1:A:344:THR:N	2.79	0.45
1:A:161:SER:C	1:A:163:LEU:H	2.19	0.45
1:A:134:ARG:HG2	1:A:136:TYR:CZ	2.51	0.45
1:A:230:THR:O	1:A:233:ARG:HD2	2.16	0.45
1:A:278:LEU:HD22	1:A:300:LEU:HG	1.99	0.45
1:A:368:ILE:HG22	1:A:369:ALA:N	2.32	0.45
1:A:231:ASP:C	1:A:232:VAL:HG23	2.36	0.45
1:A:383:LEU:HB2	1:A:388:ILE:CG1	2.47	0.45
1:A:352:ASP:C	1:A:352:ASP:OD1	2.54	0.45
1:A:585:THR:HG22	1:A:586:THR:N	2.32	0.45
1:A:571:VAL:HG12	1:A:572:GLU:O	2.17	0.45
1:A:125:VAL:HG12	1:A:126:ASP:N	2.31	0.45
1:A:478:ALA:HB3	1:A:494:VAL:O	2.16	0.45
1:A:184:GLN:HB2	1:A:309:ARG:CB	2.47	0.45
1:A:165:PRO:CA	1:A:320:VAL:HG11	2.47	0.45
1:A:364:ILE:HD12	1:A:364:ILE:H	1.81	0.45
1:A:544:LYS:HA	1:A:567:ASP:OD2	2.17	0.44
1:A:175:MET:CE	1:A:306:LEU:HD11	2.47	0.44
1:A:198:VAL:HG23	1:A:297:LEU:HA	1.99	0.44
1:A:261:VAL:O	1:A:262:GLU:C	2.54	0.44
1:A:482:GLN:HE22	1:A:586:THR:CG2	2.20	0.44
1:A:588:LEU:C	1:A:590:ALA:N	2.70	0.44
1:A:198:VAL:HG13	1:A:199:PRO:HD2	1.99	0.44
1:A:186:ARG:HH21	1:A:252:HIS:CD2	2.36	0.44
1:A:516:TRP:O	1:A:517:THR:C	2.54	0.44
1:A:133:ARG:HG3	1:A:133:ARG:O	2.17	0.44
1:A:541:LEU:HD13	1:A:569:LEU:CD1	2.48	0.43
1:A:541:LEU:CD2	1:A:569:LEU:HG	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:GLU:CG	1:A:416:VAL:HG21	2.48	0.43
1:A:237:GLN:HB3	1:A:238:PRO:CD	2.49	0.43
1:A:212:TRP:HA	1:A:213:PRO:HD2	1.89	0.43
1:A:259:ARG:HG3	1:A:272:THR:O	2.19	0.43
1:A:198:VAL:HG12	1:A:199:PRO:O	2.18	0.43
1:A:303:ALA:O	1:A:304:LEU:HD23	2.18	0.43
1:A:579:VAL:HG12	1:A:580:ALA:N	2.33	0.43
1:A:484:THR:HG22	1:A:484:THR:O	2.19	0.43
1:A:350:MET:HE3	1:A:409:THR:N	2.33	0.43
1:A:335:ALA:HB2	1:A:340:GLU:OE1	2.18	0.43
1:A:314:GLY:C	1:A:316:THR:N	2.71	0.43
1:A:300:LEU:HA	1:A:300:LEU:HD23	1.70	0.43
1:A:405:ASN:C	1:A:407:GLU:N	2.73	0.43
1:A:520:THR:HG23	1:A:523:GLY:CA	2.49	0.43
1:A:230:THR:CG2	1:A:231:ASP:N	2.82	0.42
1:A:330:ARG:HE	1:A:330:ARG:HB3	1.63	0.42
1:A:478:ALA:CB	1:A:495:SER:CA	2.91	0.42
1:A:532:TYR:N	1:A:532:TYR:CD2	2.86	0.42
1:A:532:TYR:HD2	1:A:532:TYR:N	2.17	0.42
1:A:396:PHE:HB3	1:A:413:TYR:O	2.19	0.42
1:A:329:HIS:HB2	1:A:436:SER:OG	2.19	0.42
1:A:136:TYR:CZ	1:A:175:MET:HA	2.54	0.42
1:A:524:ARG:HB3	1:A:525:PRO:HD2	2.01	0.42
1:A:503:VAL:O	1:A:503:VAL:HG12	2.19	0.42
1:A:491:PRO:HG3	1:A:583:THR:H	1.84	0.42
1:A:471:LEU:HB3	1:A:473:LEU:HD21	2.01	0.42
1:A:527:SER:CB	1:A:604:HIS:HE1	2.32	0.42
1:A:539:LEU:HA	1:A:539:LEU:HD23	1.73	0.42
1:A:222:VAL:HG13	1:A:227:ILE:HD11	2.02	0.42
1:A:366:ARG:HA	1:A:399:ARG:NH2	2.35	0.42
1:A:165:PRO:HA	1:A:320:VAL:HG11	2.02	0.42
1:A:155:LEU:HD11	1:A:280:ILE:HG23	2.02	0.42
1:A:561:TYR:O	1:A:562:ASN:HB2	2.19	0.42
1:A:343:THR:HG22	1:A:344:THR:N	2.34	0.41
1:A:545:LEU:HD21	1:A:569:LEU:HD21	2.02	0.41
1:A:534:LYS:HB2	1:A:536:PHE:CE1	2.35	0.41
1:A:349:PHE:CE2	1:A:400:PRO:HD3	2.54	0.41
1:A:246:ILE:HA	1:A:247:PRO:HD2	1.89	0.41
1:A:547:PHE:O	1:A:548:TRP:CE3	2.73	0.41
1:A:563:THR:HG22	1:A:563:THR:O	2.20	0.41
1:A:412:LEU:O	1:A:425:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:GLU:C	1:A:551:GLY:H	2.23	0.41
1:A:520:THR:HG23	1:A:523:GLY:HA2	2.03	0.41
1:A:548:TRP:H	1:A:595:ILE:HG13	1.85	0.41
1:A:415:SER:H	1:A:418:ASN:HD22	1.69	0.41
1:A:173:HIS:O	1:A:173:HIS:ND1	2.54	0.41
1:A:222:VAL:CG1	1:A:227:ILE:HD11	2.51	0.41
1:A:489:THR:OG1	1:A:584:TYR:HE2	2.02	0.41
1:A:541:LEU:HD13	1:A:569:LEU:HD12	2.02	0.41
1:A:571:VAL:HG13	1:A:578:ARG:O	2.21	0.41
1:A:174:ILE:HG22	1:A:178:GLU:CD	2.41	0.41
1:A:383:LEU:HB2	1:A:388:ILE:HG12	2.02	0.41
1:A:527:SER:HB3	1:A:604:HIS:HE1	1.86	0.41
1:A:250:ARG:CG	1:A:250:ARG:NH1	2.82	0.40
1:A:586:THR:O	1:A:588:LEU:N	2.54	0.40
1:A:341:LEU:O	1:A:409:THR:HA	2.21	0.40
1:A:520:THR:CG2	1:A:523:GLY:HA2	2.50	0.40
1:A:250:ARG:O	1:A:253:TYR:HD2	2.05	0.40
1:A:149:THR:HB	1:A:376:ALA:HB1	2.03	0.40
1:A:212:TRP:N	1:A:212:TRP:CD1	2.90	0.40
1:A:128:ARG:HB3	1:A:129:GLY:H	1.65	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	479/552 (87%)	369 (77%)	72 (15%)	38 (8%)	1 19

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	295	GLY

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Mol	Chain	Res	Type
1	A	313	PRO
1	A	424	GLY
1	A	487	SER
1	A	545	LEU
1	A	565	ALA
1	A	584	TYR
1	A	127	SER
1	A	177	THR
1	A	220	THR
1	A	347	THR
1	A	486	GLY
1	A	491	PRO
1	A	492	VAL
1	A	516	TRP
1	A	587	SER
1	A	591	GLY
1	A	268	GLU
1	A	328	ARG
1	A	335	ALA
1	A	349	PHE
1	A	564	THR
1	A	574	ALA
1	A	578	ARG
1	A	174	ILE
1	A	351	LYS
1	A	476	THR
1	A	540	PRO
1	A	287	SER
1	A	353	LEU
1	A	459	SER
1	A	503	VAL
1	A	590	ALA
1	A	219	PRO
1	A	314	GLY
1	A	359	ASN
1	A	334	GLY
1	A	232	VAL

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	403/460 (88%)	351 (87%)	52 (13%)	5 32

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	ASP
1	A	134	ARG
1	A	141	SER
1	A	149	THR
1	A	168	ASP
1	A	172	THR
1	A	210	SER
1	A	215	THR
1	A	217	THR
1	A	229	SER
1	A	233	ARG
1	A	234	ILE
1	A	235	LEU
1	A	236	VAL
1	A	238	PRO
1	A	249	GLU
1	A	252	HIS
1	A	258	TRP
1	A	279	CYS
1	A	288	TYR
1	A	289	THR
1	A	290	ASN
1	A	300	LEU
1	A	301	ASP
1	A	313	PRO
1	A	315	ASN
1	A	319	ARG
1	A	333	ARG
1	A	336	ASP
1	A	352	ASP
1	A	375	LEU
1	A	396	PHE
1	A	405	ASN
1	A	417	GLU

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Mol	Chain	Res	Type
1	A	427	ILE
1	A	449	GLN
1	A	469	ASP
1	A	481	ASP
1	A	491	PRO
1	A	496	ASP
1	A	502	ASN
1	A	522	ASP
1	A	527	SER
1	A	532	TYR
1	A	539	LEU
1	A	544	LYS
1	A	549	GLU
1	A	570	LEU
1	A	581	ILE
1	A	583	THR
1	A	584	TYR
1	A	600	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	ASN
1	A	286	ASN
1	A	290	ASN
1	A	315	ASN
1	A	329	HIS
1	A	374	ASN
1	A	418	ASN
1	A	441	GLN
1	A	482	GLN
1	A	502	ASN
1	A	573	ASN
1	A	604	HIS

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, 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	483/552 (87%)	0.20	11 (2%) 64 48	93, 135, 197, 202	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	493	TYR	5.3
1	A	581	ILE	4.9
1	A	582	SER	4.6
1	A	580	ALA	3.0
1	A	492	VAL	3.0
1	A	480	TYR	3.0
1	A	569	LEU	2.9
1	A	583	THR	2.9
1	A	481	ASP	2.7
1	A	124	ASP	2.4
1	A	554	LYS	2.3

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

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.