Full wwPDB X-ray Structure Validation Report (i)

Oct 1, 2023 – 01:47 PM EDT

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PDB ID	:	4NWV
Title	:	Crystal structure of Orsay virus-like particle
Authors	:	Tao, Y.J.; Guo, Y.R.
Deposited on	:	2013-12-06
Resolution	:	3.25 Å(reported)

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
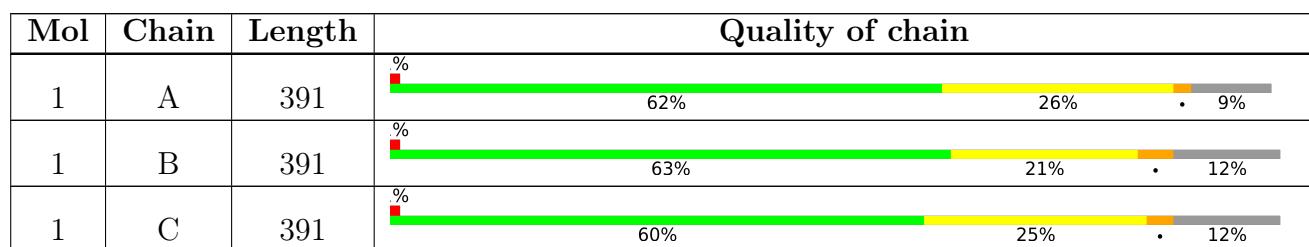
The reported resolution of this entry is 3.25 Å.

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	Percentile Ranks	Value
Rfree		0.260
Clashscore		12
Ramachandran outliers		0.7%
Sidechain outliers		9.6%
RSRZ outliers		1.1%

Worse *Better*

▌ Percentile relative to all X-ray structures

⬜ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	391	62% 26% • 9%
1	B	391	63% 21% • 12%
1	C	391	60% 25% • 12%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 8122 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
1	A	355	Total	C	N	O	S	0	0	0
			2747	1763	462	516	6			
1	C	346	Total	C	N	O	S	0	0	0
			2689	1729	448	506	6			
1	B	345	Total	C	N	O	S	0	0	0
			2683	1726	447	504	6			
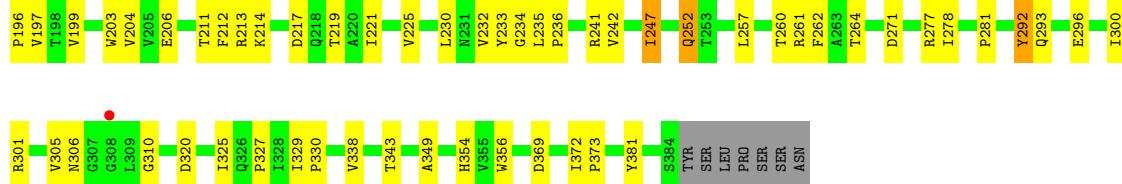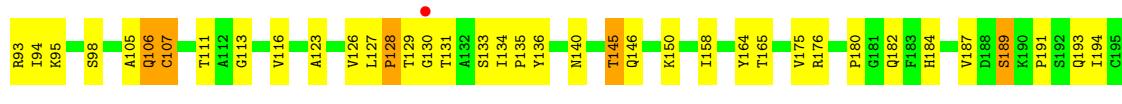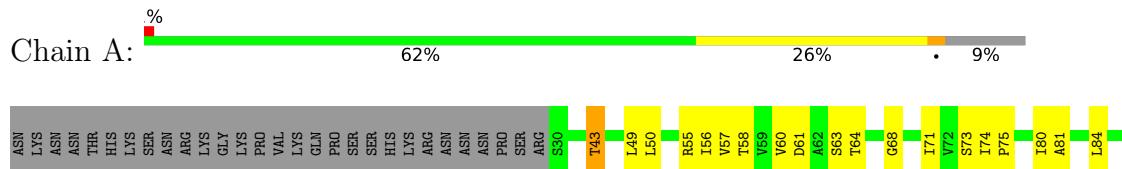
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		
2	C	1	Total	Ca	0	0
			1	1		
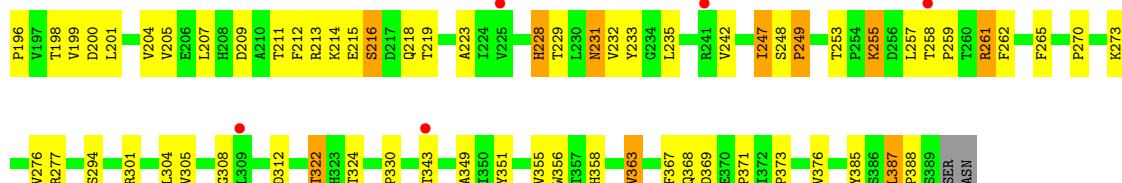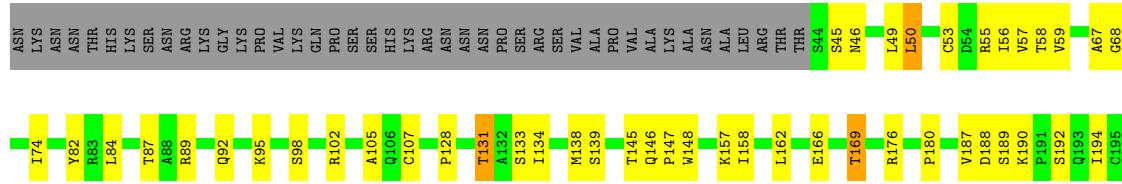
3 Residue-property plots ⓘ

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: Capsid protein

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ASN LYS ASN ASN THR HIS LYS SER ASN ARG LYS GLY LYS PRO VAL LYS GLN PRO SER SER HIS LYS ARG ASN ASN ASN PRO SER ARG SER VAL ALA PRO VAL ALA LYS ALA ASN ALA LEU ARG THR THR SER S45 L49 L50 K51 R55 I56 V57 T58 V59 V60 I71 V72

I80 A81 L84 F91 Q92 R97 S98 R102 Q106 C107 A108 T109 T110 T111 K121 D122 I134 L137 S143 F144 W149 Y164 T169 R170 L186 V187 D188 S189 Q193 P196 V197 T198 V199 D200 W203 V204 V205 E206 L207 H208 D209 A210 T211 F212

R213 K214 E215 S216 D217 Q218 I221 I224 L235 R241 I247 Q252 D256 L257 R261 F268 L269 K273 V276 R277 V285 L286 Y292 Q293 T298 H299 I300 R301 L304 V305 N306 L309 A316 N319 D320 T321 T322 H323 T324 I328

V338 T343 F346 A349 D352 F362 V363 S366 F367 Q368 I372 R383 S384 Y385 S386 L387 P388 S389 SER ASN

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	402.20Å 369.86Å 410.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.25 49.68 – 3.26	Depositor EDS
% Data completeness (in resolution range)	86.4 (50.00-3.25) 87.0 (49.68-3.26)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 3.25Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.278 , 0.279 0.259 , 0.260	Depositor DCC
R_{free} test set	20302 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	46.0	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 55.6	EDS
L-test for twinning[2]	$< |L| > = 0.52, < L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	8122	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.43	0/2823	0.65	0/3873
1	B	0.42	0/2760	0.66	0/3787
1	C	0.41	0/2766	0.64	0/3795
All	All	0.42	0/8349	0.65	0/11455

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	144	PHE	Peptide

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.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2747	0	2709	72	0
1	B	2683	0	2634	56	0
1	C	2689	0	2641	80	0
2	A	2	0	0	0	0
2	C	1	0	0	0	0
All	All	8122	0	7984	197	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 12.

All (197) 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:C:228:HIS:HB3	1:C:249:PRO:HA	1.42	1.00
1:C:228:HIS:CB	1:C:249:PRO:HA	1.99	0.91
1:C:107:CYS:SG	1:C:148:TRP:HB3	2.12	0.89
1:A:176:ARG:HG2	1:B:164:TYR:CE2	2.22	0.73
1:A:247:ILE:HD11	1:A:257:LEU:HA	1.71	0.72
1:C:247:ILE:HD11	1:C:257:LEU:HG	1.72	0.71
1:C:82:TYR:HH	1:C:385:TYR:HH	1.36	0.70
1:A:130:GLY:HA2	1:A:133:SER:OG	1.91	0.70
1:A:164:TYR:CE2	1:C:176:ARG:HG2	2.28	0.69
1:C:211:THR:HG22	1:C:212:PHE:N	2.08	0.69
1:A:43:THR:HG21	1:C:138:MET:O	1.94	0.68
1:A:158:ILE:HD13	1:A:180:PRO:HB2	1.76	0.67
1:C:247:ILE:HD13	1:C:261:ARG:HG2	1.76	0.66
1:B:49:LEU:HD12	1:B:205:VAL:O	1.95	0.66
1:C:218:GLN:HG2	1:C:371:PRO:HB3	1.77	0.66
1:B:57:VAL:HA	1:B:388:PRO:HD3	1.77	0.65
1:B:81:ALA:HB3	1:B:84:LEU:HB3	1.78	0.64
1:C:259:PRO:HB2	1:C:270:PRO:HG2	1.79	0.64
1:C:218:GLN:HG2	1:C:371:PRO:CB	2.29	0.63
1:B:109:THR:HG22	1:B:149:TRP:CD2	2.34	0.62
1:B:211:THR:HG22	1:B:212:PHE:N	2.14	0.62
1:C:67:ALA:HA	1:C:187:VAL:HG23	1.81	0.61
1:A:176:ARG:HG2	1:B:164:TYR:CZ	2.35	0.61
1:A:123:ALA:HB1	1:A:175:VAL:HG22	1.81	0.61
1:C:262:PHE:CD2	1:C:270:PRO:HG3	2.36	0.61
1:B:387:LEU:O	1:B:388:PRO:C	2.36	0.61
1:C:57:VAL:CG1	1:C:199:VAL:HB	2.32	0.60
1:C:211:THR:HG22	1:C:212:PHE:H	1.67	0.60
1:C:223:ALA:HB2	1:C:265:PHE:CZ	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:GLY:HA2	1:A:242:VAL:HG22	1.83	0.60
1:B:277:ARG:HB3	1:B:363:VAL:HG13	1.83	0.59
1:C:134:ILE:HD13	1:C:188:ASP:HA	1.83	0.59
1:C:262:PHE:CG	1:C:270:PRO:HG3	2.38	0.59
1:A:211:THR:HG22	1:A:212:PHE:N	2.18	0.59
1:C:55:ARG:HD2	1:C:200:ASP:OD2	2.03	0.57
1:C:57:VAL:HG12	1:C:199:VAL:HB	1.86	0.57
1:C:105:ALA:HB1	1:C:148:TRP:O	2.04	0.57
1:B:211:THR:HG22	1:B:212:PHE:H	1.70	0.57
1:C:257:LEU:N	1:C:257:LEU:HD12	2.19	0.56
1:C:128:PRO:HG2	1:C:133:SER:HA	1.86	0.55
1:C:95:LYS:HB2	1:C:162:LEU:HD23	1.89	0.54
1:C:228:HIS:HB2	1:C:249:PRO:HA	1.88	0.54
1:B:107:CYS:HB2	1:B:111:THR:HG21	1.89	0.54
1:A:57:VAL:HG12	1:A:199:VAL:HB	1.90	0.54
1:A:75:PRO:O	1:A:80:ILE:HD11	2.07	0.54
1:C:55:ARG:CD	1:C:200:ASP:OD2	2.55	0.54
1:C:387:LEU:HD23	1:C:388:PRO:HA	1.90	0.54
1:A:64:THR:HG21	1:A:225:VAL:HG23	1.90	0.53
1:B:58:THR:HG23	1:B:387:LEU:HB2	1.89	0.53
1:B:286:LEU:HB3	1:B:346:PHE:CD1	2.44	0.53
1:A:277:ARG:NH1	1:A:369:ASP:OD1	2.42	0.53
1:C:305:VAL:HG21	1:C:312:ASP:HB2	1.90	0.53
1:B:213:ARG:HE	1:B:214:LYS:H	1.55	0.53
1:C:49:LEU:HD12	1:C:205:VAL:O	2.09	0.52
1:C:277:ARG:HB3	1:C:363:VAL:HG13	1.92	0.52
1:C:231:ASN:HD21	1:C:248:SER:HB2	1.73	0.52
1:A:194:ILE:HG22	1:A:196:PRO:HD3	1.92	0.52
1:A:330:PRO:HG3	1:A:349:ALA:HB2	1.92	0.52
1:A:165:THR:OG1	1:A:213:ARG:NH2	2.43	0.51
1:A:123:ALA:O	1:B:170:ARG:NH1	2.44	0.51
1:A:305:VAL:HG12	1:A:310:GLY:HA3	1.92	0.51
1:C:56:ILE:CG1	1:C:201:LEU:HB2	2.40	0.51
1:B:80:ILE:HD12	1:B:80:ILE:O	2.11	0.51
1:C:187:VAL:HG23	1:C:187:VAL:O	2.10	0.51
1:C:50:LEU:HD11	1:C:87:THR:HG21	1.91	0.51
1:C:211:THR:CG2	1:C:212:PHE:N	2.73	0.51
1:C:294:SER:HB3	1:B:352:ASP:OD2	2.11	0.51
1:B:276:VAL:HG11	1:B:362:PHE:HB3	1.92	0.51
1:B:304:LEU:HD23	1:B:304:LEU:H	1.75	0.50
1:B:109:THR:HG22	1:B:149:TRP:CE3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:ASN:ND2	1:B:321:THR:HB	2.27	0.50
1:A:74:ILE:HD12	1:A:80:ILE:HD13	1.94	0.50
1:C:92:GLN:HE21	1:C:211:THR:HB	1.77	0.50
1:B:111:THR:HB	1:B:193:GLN:HG2	1.91	0.50
1:B:55:ARG:HD3	1:B:200:ASP:OD1	2.11	0.50
1:B:276:VAL:CG1	1:B:362:PHE:HB3	2.42	0.49
1:A:232:VAL:HG23	1:A:356:TRP:HZ3	1.76	0.49
1:B:56:ILE:HG23	1:B:80:ILE:HG12	1.94	0.49
1:C:134:ILE:CD1	1:C:188:ASP:HA	2.42	0.49
1:A:211:THR:HG22	1:A:212:PHE:H	1.78	0.49
1:A:217:ASP:HA	1:A:373:PRO:HA	1.95	0.49
1:C:247:ILE:HD12	1:C:255:LYS:O	2.13	0.49
1:A:252:GLN:HE21	1:A:252:GLN:N	2.10	0.49
1:C:146:GLN:HG3	1:C:147:PRO:HD2	1.95	0.49
1:C:242:VAL:HG12	1:C:351:TYR:CD2	2.47	0.48
1:C:89:ARG:NE	1:C:215:GLU:HG3	2.28	0.48
1:A:140:ASN:HD21	1:B:211:THR:HG23	1.79	0.48
1:C:258:THR:N	1:C:259:PRO:HA	2.29	0.48
1:B:134:ILE:HG12	1:B:186:LEU:HD23	1.95	0.48
1:A:128:PRO:HG2	1:A:136:TYR:CD2	2.49	0.47
1:C:166:GLU:OE1	1:C:213:ARG:HG2	2.13	0.47
1:C:223:ALA:HB3	1:C:358:HIS:HA	1.96	0.47
1:A:235:LEU:HB3	1:A:236:PRO:HD3	1.96	0.47
1:A:260:THR:O	1:A:264:THR:HG23	2.14	0.47
1:C:258:THR:OG1	1:C:261:ARG:NH1	2.46	0.47
1:B:92:GLN:NE2	1:B:211:THR:OG1	2.47	0.47
1:A:63:SER:HA	1:A:191:PRO:HG2	1.96	0.47
1:A:73:SER:HB3	1:A:184:HIS:CD2	2.50	0.47
1:C:128:PRO:O	1:C:133:SER:HB3	2.14	0.47
1:C:214:LYS:HB3	1:C:216:SER:N	2.30	0.47
1:B:134:ILE:CD1	1:B:188:ASP:HA	2.45	0.47
1:A:106:GLN:CG	1:A:196:PRO:HG2	2.45	0.47
1:C:194:ILE:HG22	1:C:196:PRO:HD3	1.97	0.47
1:A:105:ALA:HB1	1:A:107:CYS:SG	2.55	0.46
1:A:116:VAL:HG21	1:A:134:ILE:HG23	1.96	0.46
1:A:232:VAL:HG23	1:A:356:TRP:CZ3	2.50	0.46
1:C:53:CYS:HA	1:C:201:LEU:O	2.14	0.46
1:A:49:LEU:C	1:A:49:LEU:HD23	2.34	0.46
1:B:108:ALA:O	1:B:111:THR:CG2	2.64	0.46
1:B:292:TYR:CD2	1:B:292:TYR:C	2.88	0.46
1:C:232:VAL:HG23	1:C:356:TRP:CZ3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:TYR:HB2	1:B:338:VAL:HG12	1.96	0.46
1:C:211:THR:CG2	1:C:212:PHE:H	2.29	0.46
1:B:366:SER:C	1:B:367:PHE:O	2.48	0.46
1:C:74:ILE:O	1:C:74:ILE:HG23	2.16	0.46
1:B:247:ILE:HD12	1:B:261:ARG:HB3	1.96	0.46
1:A:111:THR:HG22	1:A:193:GLN:HB2	1.97	0.46
1:A:126:VAL:HG12	1:B:169:THR:HB	1.97	0.46
1:C:330:PRO:HG3	1:C:349:ALA:HB2	1.98	0.45
1:B:91:PHE:CG	1:B:207:LEU:HB3	2.51	0.45
1:A:128:PRO:HG2	1:A:136:TYR:CG	2.51	0.45
1:C:59:VAL:HA	1:C:198:THR:HG22	1.98	0.45
1:B:108:ALA:O	1:B:111:THR:HG23	2.16	0.45
1:A:271:ASP:OD1	1:A:381:TYR:CE1	2.69	0.45
1:B:268:PHE:HB3	1:B:383:ARG:HG3	1.99	0.45
1:C:242:VAL:HG12	1:C:351:TYR:HD2	1.82	0.45
1:A:194:ILE:HD12	1:A:194:ILE:H	1.81	0.45
1:B:50:LEU:HB3	1:B:203:TRP:HZ3	1.82	0.44
1:B:51:LYS:HG2	1:B:204:VAL:HG22	1.99	0.44
1:A:50:LEU:HB3	1:A:203:TRP:HZ3	1.82	0.44
1:B:323:HIS:O	1:B:368:GLN:NE2	2.50	0.44
1:A:94:ILE:HB	1:A:165:THR:HG22	1.99	0.44
1:B:137:LEU:CD2	1:B:186:LEU:HD22	2.48	0.44
1:A:71:ILE:CD1	1:A:197:VAL:HG21	2.48	0.44
1:A:93:ARG:HH11	1:A:93:ARG:HG2	1.83	0.44
1:C:169:THR:HG21	1:C:213:ARG:CZ	2.47	0.44
1:C:301:ARG:CZ	1:C:367:PHE:HE2	2.30	0.44
1:C:45:SER:OG	1:C:46:ASN:N	2.51	0.44
1:A:292:TYR:C	1:A:292:TYR:CD2	2.91	0.43
1:A:301:ARG:NH1	1:A:325:ILE:O	2.50	0.43
1:A:330:PRO:HG3	1:A:349:ALA:CB	2.48	0.43
1:A:56:ILE:HD12	1:A:56:ILE:HA	1.90	0.43
1:B:97:ARG:HH11	1:B:97:ARG:HG2	1.82	0.43
1:A:146:GLN:HG3	1:A:150:LYS:HB2	2.00	0.43
1:A:257:LEU:HD22	1:A:262:PHE:HB2	1.99	0.43
1:B:247:ILE:CG1	1:B:257:LEU:HG	2.48	0.43
1:C:322:THR:HB	1:C:324:THR:HG22	1.99	0.43
1:C:213:ARG:HG3	1:C:215:GLU:HA	2.01	0.43
1:C:58:THR:HG23	1:C:387:LEU:HB3	2.01	0.43
1:C:373:PRO:HB2	1:C:376:VAL:HG23	2.01	0.43
1:B:57:VAL:HG22	1:B:199:VAL:HG23	2.01	0.43
1:A:305:VAL:HG13	1:A:306:ASN:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:HIS:HD2	1:A:356:TRP:CE2	2.37	0.43
1:C:92:GLN:OE1	1:B:122:ASP:HB2	2.19	0.43
1:C:102:ARG:HB2	1:C:102:ARG:NH1	2.34	0.43
1:A:281:PRO:HB3	1:A:296:GLU:HG3	2.00	0.43
1:C:158:ILE:HD12	1:C:180:PRO:HB2	2.00	0.43
1:C:229:THR:HB	1:C:356:TRP:O	2.19	0.43
1:B:316:ALA:HA	1:B:328:ILE:HG13	2.00	0.43
1:A:95:LYS:HB3	1:A:206:GLU:HB2	2.01	0.42
1:A:130:GLY:O	1:A:131:THR:C	2.58	0.42
1:A:338:VAL:HG23	1:C:235:LEU:O	2.18	0.42
1:C:68:GLY:HA3	1:C:131:THR:HA	2.00	0.42
1:C:304:LEU:HB3	1:C:308:GLY:HA2	2.01	0.42
1:B:59:VAL:HG22	1:B:198:THR:HG22	2.01	0.42
1:A:127:LEU:C	1:A:128:PRO:O	2.57	0.42
1:A:278:ILE:HD12	1:A:278:ILE:HA	1.91	0.42
1:B:299:HIS:O	1:B:316:ALA:N	2.50	0.42
1:C:262:PHE:CD2	1:C:262:PHE:C	2.92	0.42
1:B:385:TYR:OH	1:B:387:LEU:HD13	2.20	0.42
1:A:56:ILE:HG13	1:A:80:ILE:HG21	2.01	0.42
1:A:123:ALA:CB	1:A:175:VAL:HG22	2.46	0.42
1:A:116:VAL:HG22	1:A:145:THR:HB	2.02	0.42
1:A:278:ILE:HD13	1:A:300:ILE:HG13	2.02	0.42
1:C:56:ILE:CG2	1:C:74:ILE:HD13	2.50	0.42
1:B:57:VAL:HG11	1:B:72:VAL:HG22	2.02	0.42
1:C:261:ARG:HB2	1:C:261:ARG:HH11	1.85	0.41
1:C:231:ASN:ND2	1:C:233:TYR:OH	2.53	0.41
1:B:241:ARG:NH1	1:B:256:ASP:HB3	2.34	0.41
1:A:134:ILE:N	1:A:135:PRO:HD2	2.35	0.41
1:C:187:VAL:O	1:C:187:VAL:CG2	2.68	0.41
1:A:327:PRO:HB2	1:A:329:ILE:HD13	2.01	0.41
1:C:231:ASN:HB3	1:C:355:VAL:HA	2.02	0.41
1:C:367:PHE:H	1:C:367:PHE:HD1	1.68	0.41
1:B:71:ILE:HG13	1:B:72:VAL:HG23	2.02	0.41
1:A:56:ILE:HG23	1:A:74:ILE:HD11	2.03	0.41
1:A:68:GLY:O	1:A:130:GLY:HA3	2.20	0.41
1:A:113:GLY:HA2	1:A:189:SER:HB3	2.03	0.41
1:A:278:ILE:HD11	1:A:356:TRP:CE2	2.56	0.41
1:B:285:VAL:O	1:B:349:ALA:HA	2.21	0.41
1:A:305:VAL:HG12	1:A:310:GLY:CA	2.51	0.41
1:C:218:GLN:HG2	1:C:371:PRO:HB2	2.03	0.40
1:C:102:ARG:HB2	1:C:102:ARG:HH11	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:VAL:O	1:B:196:PRO:HA	2.22	0.40
1:B:269:LEU:HD12	1:B:269:LEU:HA	1.92	0.40
1:A:81:ALA:HB3	1:A:84:LEU:HB3	2.03	0.40
1:A:247:ILE:HD13	1:A:261:ARG:HD2	2.02	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	353/391 (90%)	334 (95%)	17 (5%)	2 (1%)	25	59
1	B	343/391 (88%)	324 (94%)	17 (5%)	2 (1%)	25	59
1	C	344/391 (88%)	322 (94%)	19 (6%)	3 (1%)	17	50
All	All	1040/1173 (89%)	980 (94%)	53 (5%)	7 (1%)	22	56

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	PRO
1	C	369	ASP
1	C	209	ASP
1	A	61	ASP
1	B	209	ASP
1	C	249	PRO
1	B	387	LEU

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	303/338 (90%)	278 (92%)	25 (8%)	11	36
1	B	297/338 (88%)	264 (89%)	33 (11%)	6	23
1	C	298/338 (88%)	270 (91%)	28 (9%)	8	30
All	All	898/1014 (89%)	812 (90%)	86 (10%)	8	29

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	THR
1	A	55	ARG
1	A	58	THR
1	A	60	VAL
1	A	98	SER
1	A	106	GLN
1	A	107	CYS
1	A	129	THR
1	A	145	THR
1	A	182	GLN
1	A	187	VAL
1	A	189	SER
1	A	204	VAL
1	A	214	LYS
1	A	219	THR
1	A	221	ILE
1	A	230	LEU
1	A	241	ARG
1	A	247	ILE
1	A	252	GLN
1	A	292	TYR
1	A	293	GLN
1	A	320	ASP
1	A	343	THR
1	A	372	ILE
1	C	50	LEU
1	C	84	LEU
1	C	98	SER
1	C	131	THR
1	C	139	SER

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Mol	Chain	Res	Type
1	C	145	THR
1	C	157	LYS
1	C	169	THR
1	C	189	SER
1	C	190	LYS
1	C	192	SER
1	C	204	VAL
1	C	207	LEU
1	C	216	SER
1	C	219	THR
1	C	228	HIS
1	C	231	ASN
1	C	247	ILE
1	C	253	THR
1	C	255	LYS
1	C	261	ARG
1	C	273	LYS
1	C	276	VAL
1	C	322	THR
1	C	343	THR
1	C	363	VAL
1	C	368	GLN
1	C	387	LEU
1	B	50	LEU
1	B	80	ILE
1	B	98	SER
1	B	102	ARG
1	B	106	GLN
1	B	110	THR
1	B	111	THR
1	B	121	LYS
1	B	143	SER
1	B	169	THR
1	B	186	LEU
1	B	189	SER
1	B	193	GLN
1	B	214	LYS
1	B	216	SER
1	B	218	GLN
1	B	221	ILE
1	B	224	ILE
1	B	241	ARG

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Mol	Chain	Res	Type
1	B	252	GLN
1	B	257	LEU
1	B	273	LYS
1	B	292	TYR
1	B	293	GLN
1	B	298	THR
1	B	301	ARG
1	B	304	LEU
1	B	320	ASP
1	B	324	THR
1	B	343	THR
1	B	363	VAL
1	B	368	GLN
1	B	372	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	140	ASN
1	A	184	HIS
1	A	252	GLN
1	A	319	ASN
1	A	354	HIS
1	C	182	GLN
1	C	231	ASN
1	C	326	GLN
1	B	140	ASN
1	B	228	HIS
1	B	244	HIS
1	B	319	ASN
1	B	368	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 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 ⓘ

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(Å²)	Q<0.9
1	A	355/391 (90%)	0.11	3 (0%)	86	86	15, 39, 82, 185	0
1	B	345/391 (88%)	0.15	4 (1%)	79	77	14, 43, 84, 127	0
1	C	346/391 (88%)	0.25	5 (1%)	75	74	15, 47, 95, 162	0
All	All	1046/1173 (89%)	0.17	12 (1%)	80	80	14, 43, 91, 185	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	309	LEU	3.7
1	C	343	THR	2.6
1	C	258	THR	2.5
1	A	130	GLY	2.5
1	B	306	ASN	2.4
1	B	235	LEU	2.4
1	A	308	GLY	2.3
1	B	218	GLN	2.2
1	C	309	LEU	2.2
1	C	225	VAL	2.2
1	A	253	THR	2.1
1	C	241	ARG	2.1

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 monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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	901	1/1	0.83	0.29	94,94,94,94	0
2	CA	A	902	1/1	0.89	0.27	80,80,80,80	0
2	CA	C	901	1/1	0.90	0.13	73,73,73,73	0

6.5 Other polymers ⓘ

There are no such residues in this entry.