



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 02:07 pm BST

PDB ID : 3VBR
Title : Crystal structure of formaldehyde treated empty human Enterovirus 71 particle (room temperature)
Authors : Wang, X.; Peng, W.; Ren, J.; Hu, Z.; Xu, J.; Lou, Z.; Li, X.; Yin, W.; Shen, X.; Porta, C.; Walter, T.S.; Evans, G.; Axford, D.; Owen, R.; Rowlands, D.J.; Wang, J.; Stuart, D.I.; Fry, E.E.; Rao, Z.
Deposited on : 2012-01-02
Resolution : 3.80 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 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	:	2.11
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)	:	2.11

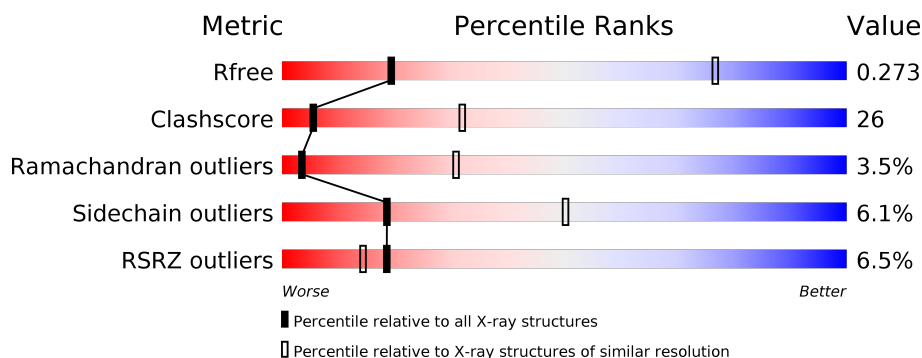
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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 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 $\leq 5\%$. 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	225	<div> <div>2%</div> <div> <div></div> <div>51%</div> <div>42%</div> <div>• •</div> </div> </div>
2	B	237	<div> <div>12%</div> <div> <div></div> <div>52%</div> <div>43%</div> <div>5%</div> </div> </div>
3	C	239	<div> <div>5%</div> <div> <div></div> <div>55%</div> <div>38%</div> <div>7%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5397 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 Genome Polyprotein, capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1724	1107	290	316	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	225	MET	CYS	SEE REMARK 999	UNP B2ZUN0

- Molecule 2 is a protein called Genome Polyprotein, capsid protein VP0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	237	Total	C	N	O	S	0	0	0
			1834	1179	301	346	8			

- Molecule 3 is a protein called Genome Polyprotein, capsid protein VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	239	Total	C	N	O	S	0	0	0
			1839	1182	306	340	11			

These plots are drawn for all protein, RNA and DNA 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.

- Chain A:
-
- 2% 51% 42%
- R166 E167 S168 L169 A170 W171 M176 P177 S178 V179 F180 V181 K182 L183 S184 D185 Q189 M195 S196 P197 Y201 Q202 W203 F204 Y205 D206 G207 T210 PHE GLY GLU HIS LYS GLN GLU K218 D219 L220 G223 A224 W225 K226 N227 N228 M229 M230 G231 T232 P233 S234 T237 V238 Q239 K242 S243 K244 Y245 P246 V249 R250 I251 Y252 M253 R254 M255 K256 R259 A260 W261 I262 P263 R264 P265 D266 R267 N270 N276 P277 N278 G281 P286 A289 S290 I294 L297

- Chain B:
-
- | Node | Category |
|------|----------|
| Q230 | Green |
| Q231 | Green |
| Q232 | Green |
| Q233 | Green |
| Q234 | Green |
| L235 | Green |
| D236 | Green |
| D237 | Green |
| G238 | Green |
| L239 | Green |
| P240 | Green |
| L241 | Green |
| S242 | Green |
| Q243 | Green |
| Q244 | Green |
| T245 | Green |
| V246 | Green |
| L252 | Green |
| M257 | Green |
| M258 | Green |
| C259 | Green |
| A260 | Green |
| L263 | Green |
| L267 | Green |
| M268 | Green |
| F272 | Green |
| M277 | Green |
| H278 | Green |
| C279 | Green |
| M280 | Green |
| F281 | Green |
| G282 | Green |
| L283 | Green |
| L284 | Green |
| V285 | Green |
| L286 | Green |
| P287 | Green |
| L291 | Green |
| D292 | Green |
| I301 | Green |
| F302 | Green |
| I303 | Green |
| T304 | Green |
| I305 | Green |
| E313 | Green |
| F314 | Green |
| L317 | Green |
| F318 | Green |
| T156 | Green |
| E157 | Green |
| G158 | Green |
| G159 | Green |
| G162 | Green |
| G163 | Green |
| M164 | Green |
| A165 | Green |
| H168 | Green |
| Y169 | Green |
| L170 | Green |
| Y171 | Green |
| R172 | Green |
| S173 | Green |
| G174 | Green |
| Q180 | Green |
| S184 | Green |
| K185 | Green |
| F186 | Green |
| H187 | Green |
| Q188 | Green |
| L191 | Green |
| V195 | Green |
| L196 | Green |
| P197 | Green |
| E198 | Green |
| L201 | Green |
| G202 | Green |
| T203 | Green |
| V204 | Green |
| A205 | Green |
| G206 | Green |
| G207 | Green |
| T208 | Green |
| G209 | Green |
| T210 | Green |
| E211 | Green |
| T213 | Green |
| H214 | Green |
| P215 | Green |
| P216 | Green |
| K218 | Green |
| Q219 | Green |
| T220 | Green |
| Q221 | Green |
| P222 | Green |
| G223 | Green |
| A224 | Green |
| D225 | Green |
| G226 | Green |
| E227 | Green |
| V82 | Green |
| L85 | Green |
| T86 | Green |
| M89 | Green |
| S90 | Green |
| T91 | Green |
| I92 | Green |
| T93 | Green |
| T94 | Green |
| Q95 | Green |
| E96 | Green |
| A97 | Green |
| A98 | Green |
| V102 | Green |
| P108 | Green |
| C111 | Green |
| S112 | Green |
| D113 | Green |
| S114 | Green |
| D115 | Green |
| A116 | Green |
| T117 | Green |
| A118 | Green |
| V119 | Green |
| D120 | Green |
| K121 | Green |
| P122 | Green |
| T123 | Green |
| R124 | Green |
| P125 | Green |
| D126 | Green |
| V127 | Green |
| S128 | Green |
| V129 | Green |
| H130 | Green |
| R131 | Green |
| F132 | Green |
| L135 | Green |
| D136 | Green |
| T137 | Green |
| K138 | Green |
| L139 | Green |
| W140 | Green |
| E141 | Green |
| K145 | Green |
| Y148 | Green |
| W149 | Green |
| K150 | Green |
| F151 | Green |
| V154 | Green |
| L155 | Green |
| L85 | Red |
| A97 | Red |
| P108 | Orange |
| C111 | Red |
| S112 | Red |
| D113 | Red |
| S114 | Red |
| D115 | Red |
| A116 | Red |
| T117 | Red |
| A118 | Red |
| V119 | Red |
| D120 | Red |
| K121 | Red |
| P122 | Red |
| T123 | Red |
| R124 | Red |
| P125 | Red |
| D126 | Red |
| V127 | Red |
| H130 | Red |
| R131 | Red |
| F132 | Red |
| L135 | Red |
| D136 | Red |
| T137 | Red |
| K138 | Red |
| L139 | Red |
| W140 | Red |
| E141 | Red |
| K145 | Red |
| Y148 | Red |
| W149 | Red |
| K150 | Red |
| F151 | Red |
| V154 | Red |
| L155 | Red |

- Chain C:



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 ₂ 3 2	Depositor
Cell constants a, b, c, α , β , γ	354.90 Å 354.90 Å 354.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.70 – 3.80 49.70 – 3.80	Depositor EDS
% Data completeness (in resolution range)	90.3 (49.70-3.80) 90.3 (49.70-3.80)	Depositor EDS
R_{merge}	0.44	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 3.77 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.257 , 0.284 0.256 , 0.273	Depositor DCC
R_{free} test set	683 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	102.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 114.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	5397	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.40% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.46	0/1776	0.69	0/2419
2	B	0.49	0/1889	0.68	0/2592
3	C	0.47	0/1891	0.70	0/2586
All	All	0.47	0/5556	0.69	0/7597

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	1724	0	1688	101	0
2	B	1834	0	1774	111	0
3	C	1839	0	1814	106	0
All	All	5397	0	5276	276	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 26.

All (276) 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:229:MET:HE2	1:A:231:GLY:H	1.11	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:GLY:HA3	2:B:204:VAL:HG13	1.35	1.03
2:B:124:ARG:HG2	2:B:313:GLU:HG2	1.48	0.93
3:C:66:MET:HE2	3:C:69:LEU:HD11	1.54	0.87
1:A:104:ASN:O	1:A:166:ARG:HD2	1.75	0.85
1:A:229:MET:HE2	1:A:231:GLY:N	1.93	0.80
1:A:281:GLY:CA	2:B:204:VAL:HG13	2.10	0.80
3:C:105:CYS:HA	3:C:226:MET:HE1	1.64	0.80
2:B:85:LEU:HD21	2:B:94:THR:CG2	2.12	0.80
3:C:6:LEU:HD13	3:C:10:THR:HG21	1.65	0.78
2:B:243:GLN:HA	3:C:51:THR:HG22	1.66	0.77
3:C:144:LYS:HD3	3:C:148:THR:HG21	1.63	0.77
1:A:156:VAL:HG22	1:A:232:THR:HB	1.66	0.77
3:C:9:GLY:O	3:C:12:GLN:HG2	1.86	0.76
1:A:197:PRO:HA	3:C:31:THR:HG21	1.69	0.74
2:B:252:ILE:HA	2:B:257:ASN:HD21	1.51	0.74
3:C:58:VAL:HG23	3:C:59:PRO:HD3	1.69	0.74
2:B:138:LYS:HE3	2:B:225:ASP:O	1.87	0.73
3:C:42:ASN:O	3:C:45:GLU:HG3	1.88	0.73
3:C:105:CYS:HA	3:C:226:MET:CE	2.19	0.73
2:B:188:GLN:NE2	3:C:209:PRO:HB2	2.04	0.72
2:B:128:SER:O	2:B:131:ARG:HG2	1.89	0.72
1:A:297:LEU:H	1:A:297:LEU:HD12	1.56	0.71
3:C:167:LEU:HD12	3:C:168:VAL:H	1.55	0.71
3:C:66:MET:HE2	3:C:69:LEU:CD1	2.21	0.71
2:B:90:SER:HB2	2:B:132:PHE:HB2	1.72	0.71
2:B:240:PRO:HG3	2:B:243:GLN:NE2	2.07	0.70
3:C:188:TYR:O	3:C:189:TYR:HD2	1.74	0.70
2:B:85:LEU:HD21	2:B:94:THR:HG22	1.72	0.70
2:B:241:ILE:HG21	3:C:66:MET:HE1	1.77	0.67
3:C:188:TYR:O	3:C:189:TYR:CD2	2.48	0.66
1:A:76:ALA:O	1:A:79:THR:HG23	1.95	0.66
3:C:142:LEU:HD23	3:C:143:PRO:O	1.95	0.66
3:C:73:VAL:HA	3:C:198:TYR:OH	1.95	0.66
1:A:141:THR:HB	1:A:142:PRO:HD2	1.78	0.65
1:A:75:THR:HG22	3:C:225:THR:HG22	1.77	0.65
1:A:112:ASP:OD1	1:A:114:THR:HG22	1.96	0.65
1:A:294:ILE:HD11	3:C:55:VAL:HG12	1.80	0.63
1:A:226:PRO:C	1:A:228:ASN:H	2.02	0.63
1:A:152:GLN:HG3	1:A:180:PHE:CE2	2.34	0.63
1:A:117:ALA:HB1	3:C:236:LEU:HD23	1.80	0.63
3:C:235:ILE:C	3:C:236:LEU:HD12	2.19	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:190:THR:O	3:C:192:GLY:N	2.33	0.62
2:B:82:VAL:N	2:B:96:GLU:HG3	2.14	0.62
2:B:267:ILE:HG12	3:C:37:PRO:HG2	1.82	0.61
2:B:233:TYR:HA	3:C:66:MET:HE1	1.80	0.61
2:B:191:LEU:HD23	2:B:287:PRO:HA	1.83	0.61
1:A:276:ASN:HB2	1:A:277:PRO:HD2	1.83	0.61
3:C:180:HIS:CD2	3:C:181:ALA:H	2.18	0.61
3:C:138:PRO:HB3	3:C:190:THR:HA	1.83	0.61
3:C:167:LEU:HD12	3:C:168:VAL:N	2.16	0.61
2:B:187:HIS:CD2	2:B:301:ILE:HD11	2.36	0.60
2:B:85:LEU:HD23	2:B:85:LEU:H	1.67	0.60
3:C:54:GLU:HG2	3:C:69:LEU:HD23	1.82	0.60
1:A:254:ARG:NH2	1:A:256:LYS:HD3	2.16	0.60
2:B:204:VAL:HG22	2:B:231:HIS:HE1	1.67	0.60
3:C:204:VAL:HG22	3:C:205:PRO:HD2	1.82	0.59
3:C:65:LEU:O	3:C:68:ARG:HG3	2.03	0.59
2:B:268:ASN:OD1	2:B:278:HIS:HE1	1.85	0.58
3:C:133:ILE:HG12	3:C:196:ILE:HG12	1.85	0.58
1:A:267:ARG:HD2	2:B:238:GLY:O	2.02	0.58
1:A:254:ARG:NH1	3:C:18:ASP:HA	2.18	0.58
2:B:164:ASN:O	2:B:168:HIS:HB2	2.04	0.58
1:A:125:LEU:HD23	1:A:126:PHE:CE2	2.39	0.58
1:A:97:LEU:HD11	1:A:246:PRO:HD3	1.86	0.58
2:B:203:THR:HG23	2:B:219:GLN:HE22	1.68	0.57
3:C:185:VAL:O	3:C:185:VAL:HG23	2.04	0.57
3:C:58:VAL:H	3:C:59:PRO:HD2	1.68	0.57
1:A:270:ASN:HA	3:C:235:ILE:HG23	1.86	0.57
2:B:117:THR:CG2	2:B:120:ASP:HB3	2.35	0.57
1:A:254:ARG:HH21	1:A:256:LYS:HD3	1.68	0.56
2:B:148:TYR:HB3	2:B:284:LEU:HD12	1.86	0.56
2:B:85:LEU:N	2:B:85:LEU:HD23	2.20	0.56
2:B:233:TYR:HA	3:C:66:MET:CE	2.34	0.56
1:A:112:ASP:CG	1:A:114:THR:HG22	2.25	0.56
1:A:294:ILE:HD12	3:C:56:ASN:HA	1.87	0.56
1:A:229:MET:CE	1:A:231:GLY:H	2.02	0.56
1:A:104:ASN:HA	1:A:242:LYS:NZ	2.21	0.56
3:C:180:HIS:CG	3:C:181:ALA:H	2.24	0.56
2:B:125:PRO:HB3	2:B:129:VAL:HG21	1.88	0.55
3:C:105:CYS:CA	3:C:226:MET:HE1	2.36	0.55
1:A:229:MET:CE	1:A:230:MET:H	2.20	0.55
2:B:148:TYR:CB	2:B:284:LEU:HD12	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ARG:NH2	1:A:237:THR:OG1	2.39	0.55
2:B:185:LYS:HD3	3:C:125:PHE:CE1	2.41	0.55
2:B:135:LEU:HD23	2:B:135:LEU:N	2.21	0.55
2:B:156:THR:HG22	2:B:165:ALA:HB1	1.90	0.54
1:A:171:TRP:CH2	1:A:234:SER:HB3	2.42	0.54
1:A:281:GLY:HA3	2:B:204:VAL:CG1	2.24	0.54
3:C:144:LYS:CD	3:C:148:THR:HG21	2.34	0.54
1:A:290:SER:OG	3:C:68:ARG:NH2	2.41	0.54
1:A:112:ASP:OD2	1:A:114:THR:HG22	2.08	0.54
2:B:168:HIS:CD2	2:B:314:PHE:HB3	2.43	0.54
3:C:227:LYS:O	3:C:228:LEU:HB2	2.07	0.53
1:A:156:VAL:O	1:A:156:VAL:HG23	2.08	0.53
1:A:156:VAL:CG2	1:A:156:VAL:O	2.56	0.53
2:B:203:THR:CG2	2:B:219:GLN:HE22	2.22	0.53
3:C:56:ASN:O	3:C:68:ARG:HA	2.09	0.52
2:B:154:VAL:HG23	2:B:224:ALA:HA	1.91	0.52
1:A:237:THR:HG21	1:A:243:SER:HB2	1.92	0.52
3:C:221:GLN:HB3	3:C:223:ASN:OD1	2.09	0.52
1:A:262:ILE:HG21	2:B:197:PRO:HG2	1.92	0.52
2:B:137:THR:HG23	2:B:303:ILE:O	2.10	0.52
3:C:52:ILE:HA	3:C:217:LEU:HD23	1.91	0.52
2:B:126:ASP:O	2:B:127:VAL:O	2.28	0.51
3:C:71:PHE:HE1	3:C:214:ILE:HD12	1.75	0.51
1:A:127:THR:HG23	1:A:264:ARG:NH2	2.25	0.51
1:A:117:ALA:CB	3:C:236:LEU:HD23	2.40	0.51
1:A:205:TYR:O	1:A:223:GLY:HA2	2.10	0.51
2:B:137:THR:OG1	2:B:304:THR:HG23	2.09	0.51
2:B:222:PRO:HB3	2:B:227:PHE:HB2	1.90	0.51
3:C:58:VAL:HG23	3:C:59:PRO:CD	2.39	0.51
1:A:265:PRO:HB2	2:B:239:ILE:HB	1.92	0.51
1:A:238:VAL:HG12	1:A:239:GLY:N	2.24	0.51
2:B:140:TRP:CE2	2:B:291:LEU:HB2	2.46	0.51
2:B:140:TRP:HD1	2:B:141:GLU:N	2.09	0.51
1:A:165:SER:HB2	1:A:167:GLU:OE2	2.11	0.50
2:B:145:LYS:HZ2	2:B:145:LYS:HB3	1.76	0.50
1:A:224:ALA:O	1:A:226:PRO:HD3	2.11	0.50
2:B:117:THR:HG21	2:B:120:ASP:HB3	1.93	0.50
2:B:156:THR:HG22	2:B:165:ALA:CB	2.42	0.50
1:A:181:VAL:HG23	1:A:185:ASP:HB2	1.92	0.50
2:B:184:SER:C	2:B:186:PHE:H	2.13	0.50
1:A:94:ASP:C	1:A:96:PRO:HD3	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:PRO:O	1:A:228:ASN:N	2.44	0.49
3:C:197:TRP:N	3:C:197:TRP:CD1	2.80	0.49
3:C:147:ALA:O	3:C:150:MET:HB3	2.11	0.49
1:A:123:VAL:C	1:A:125:LEU:H	2.16	0.49
1:A:152:GLN:HG3	1:A:180:PHE:CZ	2.47	0.49
3:C:171:TRP:HE1	3:C:173:SER:HB2	1.77	0.49
2:B:235:LEU:O	2:B:236:ASP:C	2.51	0.49
2:B:149:TRP:HZ3	2:B:285:VAL:CG1	2.25	0.49
3:C:14:LEU:HB3	3:C:17:ASP:HB2	1.94	0.49
2:B:172:ARG:HD2	2:B:272:PHE:CZ	2.48	0.49
2:B:119:VAL:O	2:B:121:LYS:HG2	2.13	0.49
2:B:145:LYS:NZ	2:B:145:LYS:HB3	2.27	0.49
3:C:109:THR:HB	3:C:228:LEU:CB	2.42	0.49
1:A:229:MET:HE3	1:A:230:MET:H	1.77	0.49
3:C:109:THR:HB	3:C:228:LEU:HB2	1.93	0.49
1:A:197:PRO:CA	3:C:31:THR:HG21	2.42	0.49
3:C:90:PRO:HD2	3:C:188:TYR:OH	2.13	0.49
3:C:174:ASN:O	3:C:174:ASN:OD1	2.31	0.48
3:C:70:ARG:HG2	3:C:213:TYR:CD2	2.48	0.48
1:A:104:ASN:HB2	1:A:106:TYR:CD1	2.48	0.48
2:B:155:LEU:HD23	2:B:158:THR:HB	1.96	0.48
2:B:230:GLN:O	2:B:231:HIS:CD2	2.67	0.48
1:A:195:MET:O	1:A:196:SER:O	2.31	0.48
1:A:245:TYR:CD1	1:A:245:TYR:N	2.81	0.47
1:A:95:LEU:N	1:A:96:PRO:HD3	2.28	0.47
1:A:204:PHE:CE1	1:A:264:ARG:HD3	2.50	0.47
1:A:139:ALA:HB2	1:A:249:VAL:HG22	1.96	0.47
1:A:201:TYR:HA	1:A:228:ASN:HD21	1.79	0.47
3:C:90:PRO:CG	3:C:115:LEU:HD11	2.45	0.47
1:A:289:ALA:HB3	3:C:93:ASN:HB3	1.95	0.47
1:A:163:PRO:HB3	1:A:168:SER:HB3	1.97	0.47
2:B:305:ILE:HD12	2:B:305:ILE:N	2.30	0.47
2:B:235:LEU:HD21	2:B:241:ILE:HG13	1.97	0.47
1:A:156:VAL:CG2	1:A:232:THR:HB	2.41	0.46
2:B:218:LYS:N	2:B:218:LYS:HD2	2.30	0.46
2:B:108:PRO:HB3	2:B:174:GLY:HA3	1.96	0.46
1:A:180:PHE:N	1:A:180:PHE:CD1	2.83	0.46
1:A:297:LEU:HD12	1:A:297:LEU:N	2.26	0.46
2:B:85:LEU:HD21	2:B:94:THR:HG21	1.95	0.46
3:C:176:HIS:HB2	3:C:189:TYR:CE2	2.50	0.46
1:A:201:TYR:HA	1:A:228:ASN:ND2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:GLN:HG2	3:C:21:SER:HB3	1.97	0.46
3:C:58:VAL:CG2	3:C:59:PRO:HD3	2.42	0.46
1:A:85:SER:O	1:A:86:ARG:O	2.34	0.46
1:A:108:ASN:ND2	1:A:234:SER:OG	2.49	0.46
1:A:104:ASN:HA	1:A:242:LYS:HZ2	1.81	0.46
2:B:151:PHE:O	2:B:279:CYS:HA	2.15	0.46
3:C:71:PHE:CE1	3:C:214:ILE:HB	2.51	0.45
1:A:177:PRO:HB2	3:C:24:ILE:HD11	1.98	0.45
1:A:181:VAL:CG2	1:A:185:ASP:HB2	2.47	0.45
1:A:276:ASN:OD1	1:A:278:ASN:HB2	2.16	0.45
2:B:222:PRO:HB2	2:B:226:GLY:O	2.16	0.45
3:C:93:ASN:HD22	3:C:93:ASN:N	2.13	0.45
1:A:195:MET:O	1:A:196:SER:C	2.55	0.45
1:A:218:LYS:CA	2:B:216:PRO:HA	2.47	0.45
1:A:238:VAL:CG1	1:A:239:GLY:N	2.78	0.45
3:C:105:CYS:SG	3:C:226:MET:HE1	2.57	0.45
2:B:243:GLN:O	2:B:246:VAL:HG12	2.16	0.45
2:B:171:TYR:CE2	2:B:173:SER:HB3	2.52	0.45
2:B:220:THR:HG22	2:B:221:GLN:NE2	2.31	0.45
3:C:142:LEU:C	3:C:142:LEU:HD23	2.37	0.45
2:B:195:VAL:HG13	2:B:281:PHE:CD2	2.51	0.45
2:B:125:PRO:HB3	2:B:129:VAL:CG2	2.47	0.45
2:B:241:ILE:C	2:B:243:GLN:H	2.20	0.44
3:C:109:THR:HG21	3:C:228:LEU:HD12	1.99	0.44
1:A:250:ARG:HH21	1:A:250:ARG:HG3	1.81	0.44
1:A:266:MET:O	2:B:240:PRO:HD3	2.17	0.44
2:B:185:LYS:HB3	3:C:125:PHE:HD1	1.82	0.44
2:B:148:TYR:HA	2:B:283:LEU:O	2.17	0.44
2:B:218:LYS:H	2:B:218:LYS:HD2	1.82	0.44
1:A:220:LEU:HD23	2:B:214:HIS:HD2	1.82	0.44
2:B:286:VAL:HA	2:B:287:PRO:HD3	1.85	0.44
2:B:117:THR:HG22	2:B:117:THR:O	2.18	0.44
2:B:140:TRP:NE1	2:B:291:LEU:HB2	2.32	0.44
3:C:188:TYR:O	3:C:189:TYR:HB3	2.16	0.44
1:A:123:VAL:HB	1:A:203:TRP:NE1	2.33	0.44
2:B:85:LEU:CD2	2:B:94:THR:HG22	2.44	0.44
2:B:185:LYS:HB3	3:C:125:PHE:CD1	2.53	0.44
3:C:148:THR:HA	3:C:151:LEU:HD12	1.99	0.44
3:C:56:ASN:OD1	3:C:58:VAL:HG22	2.17	0.44
1:A:226:PRO:C	1:A:228:ASN:N	2.69	0.44
1:A:88:GLY:O	1:A:252:TYR:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:ASN:OD1	2:B:278:HIS:CE1	2.67	0.44
1:A:135:PHE:O	1:A:189:GLN:HA	2.18	0.43
1:A:281:GLY:N	2:B:204:VAL:HG13	2.33	0.43
1:A:140:CYS:SG	1:A:144:GLY:HA2	2.57	0.43
2:B:188:GLN:HG3	2:B:292:ASP:HB3	2.00	0.43
2:B:96:GLU:O	2:B:97:ALA:HB2	2.17	0.43
1:A:218:LYS:HA	2:B:216:PRO:HA	2.00	0.43
1:A:135:PHE:CE1	1:A:253:MET:HB2	2.53	0.43
2:B:234:VAL:HA	2:B:239:ILE:O	2.19	0.43
1:A:120:ARG:HH11	3:C:237:GLN:HE22	1.65	0.43
1:A:207:GLY:HA3	2:B:277:ASN:O	2.19	0.43
2:B:89:ASN:HD21	2:B:131:ARG:NH1	2.16	0.43
3:C:132:LEU:C	3:C:132:LEU:HD23	2.39	0.43
2:B:168:HIS:CE1	2:B:317:LEU:HD13	2.54	0.43
2:B:241:ILE:O	2:B:243:GLN:N	2.52	0.43
2:B:198:GLU:OE2	2:B:278:HIS:NE2	2.51	0.43
3:C:144:LYS:CG	3:C:148:THR:HG21	2.49	0.43
3:C:53:LEU:CD2	3:C:95:PRO:HB3	2.49	0.43
1:A:163:PRO:HG3	1:A:170:ALA:HB3	2.00	0.43
3:C:89:ASP:HA	3:C:188:TYR:CE1	2.54	0.43
3:C:211:THR:HG22	3:C:212:ALA:N	2.34	0.43
2:B:86:THR:HG23	2:B:90:SER:O	2.18	0.43
3:C:83:CYS:HB3	3:C:196:ILE:HG22	2.00	0.43
1:A:157:PRO:HD2	1:A:176:ASN:OD1	2.19	0.42
3:C:141:PRO:O	3:C:142:LEU:C	2.57	0.42
3:C:118:THR:HG23	3:C:166:THR:OG1	2.19	0.42
2:B:245:THR:OG1	3:C:50:GLU:O	2.30	0.42
1:A:261:TRP:CD1	3:C:36:ILE:HB	2.53	0.42
2:B:184:SER:C	2:B:186:PHE:N	2.72	0.42
1:A:128:TYR:HD1	1:A:202:GLN:HB3	1.84	0.42
2:B:140:TRP:CD1	2:B:141:GLU:N	2.87	0.42
2:B:241:ILE:C	2:B:243:GLN:N	2.72	0.42
2:B:92:ILE:HG13	2:B:92:ILE:O	2.19	0.42
1:A:117:ALA:HB1	3:C:236:LEU:HB3	2.01	0.42
3:C:58:VAL:H	3:C:59:PRO:CD	2.32	0.42
3:C:92:ARG:HD3	3:C:188:TYR:CD2	2.55	0.42
3:C:85:VAL:HG22	3:C:86:PHE:N	2.34	0.42
3:C:54:GLU:HG3	3:C:98:SER:CB	2.49	0.42
2:B:156:THR:HA	2:B:162:GLY:HA2	2.00	0.42
2:B:172:ARG:HD3	2:B:313:GLU:OE2	2.20	0.42
2:B:170:LEU:HB3	2:B:272:PHE:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:71:PHE:CE1	3:C:214:ILE:HD12	2.53	0.42
2:B:148:TYR:HB3	2:B:284:LEU:CD1	2.49	0.42
3:C:61:ASN:ND2	3:C:64:SER:OG	2.53	0.42
3:C:188:TYR:O	3:C:189:TYR:CB	2.67	0.41
3:C:87:ARG:HG3	3:C:89:ASP:OD2	2.20	0.41
2:B:121:LYS:HG2	2:B:121:LYS:H	1.57	0.41
1:A:97:LEU:HD21	1:A:245:TYR:C	2.41	0.41
1:A:259:ARG:HG2	3:C:39:GLU:OE1	2.21	0.41
3:C:53:LEU:HD21	3:C:95:PRO:CB	2.51	0.41
1:A:114:THR:HG23	3:C:237:GLN:HG2	2.01	0.41
2:B:252:ILE:HD11	2:B:260:ALA:HB3	2.01	0.41
2:B:215:PRO:HA	2:B:216:PRO:HD3	1.94	0.41
1:A:286:PRO:HA	2:B:233:TYR:HE2	1.86	0.41
2:B:246:VAL:O	2:B:246:VAL:HG22	2.21	0.41
3:C:180:HIS:CG	3:C:181:ALA:N	2.88	0.41
1:A:261:TRP:CD1	3:C:39:GLU:HB2	2.56	0.41
3:C:90:PRO:CD	3:C:188:TYR:OH	2.68	0.41
1:A:155:PHE:O	1:A:177:PRO:HD2	2.20	0.40
2:B:259:CYS:SG	2:B:259:CYS:O	2.79	0.40
2:B:102:VAL:HA	2:B:263:ILE:HB	2.03	0.40
2:B:283:LEU:HD12	2:B:284:LEU:N	2.36	0.40
3:C:48:GLN:OE1	3:C:222:LYS:HA	2.21	0.40
1:A:104:ASN:HB2	1:A:106:TYR:CE1	2.55	0.40
2:B:201:ILE:HG21	2:B:219:GLN:HE21	1.86	0.40
3:C:31:THR:HA	3:C:32:PRO:HD3	1.89	0.40
1:A:181:VAL:HG22	1:A:182:LYS:O	2.22	0.40
2:B:108:PRO:CB	2:B:174:GLY:HA3	2.52	0.40
3:C:90:PRO:HG2	3:C:115:LEU:HD11	2.02	0.40
3:C:35:HIS:O	3:C:36:ILE:HD13	2.20	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	214/225 (95%)	185 (86%)	24 (11%)	5 (2%)	6	38
2	B	235/237 (99%)	196 (83%)	30 (13%)	9 (4%)	3	29
3	C	237/239 (99%)	207 (87%)	20 (8%)	10 (4%)	3	26
All	All	686/701 (98%)	588 (86%)	74 (11%)	24 (4%)	3	31

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	SER
2	B	127	VAL
2	B	159	GLY
3	C	180	HIS
3	C	188	TYR
1	A	85	SER
1	A	86	ARG
1	A	124	GLU
2	B	97	ALA
2	B	237	ALA
3	C	62	ALA
3	C	182	ARG
3	C	189	TYR
3	C	191	THR
1	A	227	ASN
2	B	98	ALA
2	B	216	PRO
3	C	72	PRO
2	B	108	PRO
2	B	242	SER
3	C	181	ALA
2	B	112	SER
3	C	58	VAL
3	C	137	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	187/193 (97%)	177 (95%)	10 (5%)	22	54
2	B	201/201 (100%)	191 (95%)	10 (5%)	24	55
3	C	199/199 (100%)	183 (92%)	16 (8%)	12	42
All	All	587/593 (99%)	551 (94%)	36 (6%)	18	50

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	ASP
1	A	100	THR
1	A	101	THR
1	A	114	THR
1	A	116	TYR
1	A	179	VAL
1	A	183	LEU
1	A	245	TYR
1	A	265	PRO
1	A	297	LEU
2	B	85	LEU
2	B	119	VAL
2	B	131	ARG
2	B	135	LEU
2	B	145	LYS
2	B	171	TYR
2	B	180	GLN
2	B	203	THR
2	B	285	VAL
2	B	304	THR
3	C	14	LEU
3	C	25	LEU
3	C	31	THR
3	C	51	THR
3	C	53	LEU
3	C	61	ASN
3	C	70	ARG
3	C	72	PRO
3	C	87	ARG
3	C	136	THR
3	C	146	ARG
3	C	178	ARG
3	C	197	TRP
3	C	204	VAL

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Mol	Chain	Res	Type
3	C	221	GLN
3	C	234	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	202	GLN
1	A	228	ASN
2	B	95	GLN
2	B	168	HIS
2	B	188	GLN
2	B	214	HIS
2	B	219	GLN
2	B	257	ASN
2	B	277	ASN
3	C	61	ASN
3	C	93	ASN
3	C	237	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 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	218/225 (96%)	-0.39	4 (1%) 68 61	70, 97, 150, 190	0
2	B	237/237 (100%)	0.19	28 (11%) 4 5	72, 118, 199, 202	0
3	C	239/239 (100%)	-0.20	13 (5%) 25 22	72, 98, 189, 202	0
All	All	694/701 (99%)	-0.13	45 (6%) 18 14	70, 102, 189, 202	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	209	GLY	8.2
3	C	184	GLY	6.6
2	B	208	THR	5.3
2	B	210	THR	5.2
3	C	183	ASP	5.0
3	C	177	TYR	5.0
2	B	205	ALA	4.9
3	C	182	ARG	4.7
3	C	181	ALA	4.6
3	C	180	HIS	4.2
3	C	186	PHE	3.9
3	C	187	ASP	3.8
2	B	211	GLU	3.7
2	B	207	GLY	3.6
2	B	120	ASP	3.5
3	C	178	ARG	3.5
3	C	176	HIS	3.5
1	A	219	ASP	3.4
3	C	189	TYR	3.3
1	A	218	LYS	3.3
2	B	113	ASP	3.3
2	B	212	ASP	3.2
3	C	179	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	206	GLY	3.2
2	B	115	ASP	3.2
2	B	121	LYS	3.1
1	A	210	THR	3.0
2	B	116	ALA	3.0
2	B	111	CYS	2.9
2	B	122	PRO	2.7
2	B	114	SER	2.7
2	B	126	ASP	2.7
2	B	117	THR	2.7
2	B	204	VAL	2.6
1	A	73	HIS	2.5
2	B	112	SER	2.5
2	B	213	THR	2.4
2	B	130	ASN	2.3
2	B	96	GLU	2.3
3	C	239	GLY	2.2
2	B	124	ARG	2.2
2	B	272	PHE	2.2
2	B	118	ALA	2.1
2	B	203	THR	2.1
2	B	123	THR	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 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.