W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:27 am GMT

PDB ID : 3VBO

Title : Crystal structure of formaldehyde treated empty human Enterovirus 71 particle (cryo at 100K)

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 : 2.88 Å(reported)

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

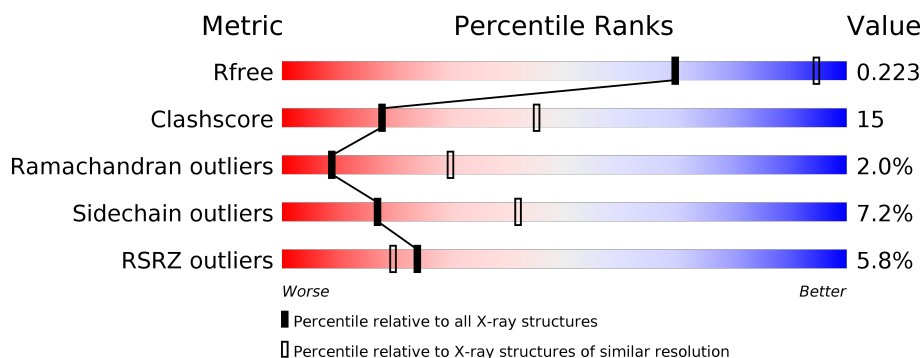|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 2.88 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		0.223
Clashscore		15
Ramachandran outliers		2.0%
Sidechain outliers		7.2%
RSRZ outliers		5.8%

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}	100719	2135 (2.90-2.86)
Clashscore	112137	2400 (2.90-2.86)
Ramachandran outliers	110173	2346 (2.90-2.86)
Sidechain outliers	110143	2349 (2.90-2.86)
RSRZ outliers	101464	2149 (2.90-2.86)

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	297	% — 49% / 22% / • / 27%
2	B	237	10% — 71% / 26% / •
3	C	239	5% — 65% / 31% / •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5466 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 VP2.

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			

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	20	Total	O	0	0
			20	20		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	23	Total 23	O 23	0	0
5	C	25	Total 25	O 25	0	0

3 Residue-property plots ⓘ

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.

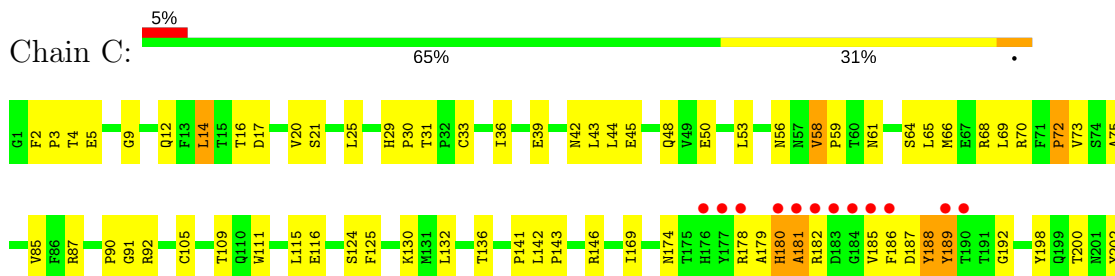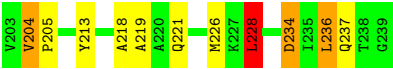• Molecule 1: Genome Polyprotein, capsid protein VP1
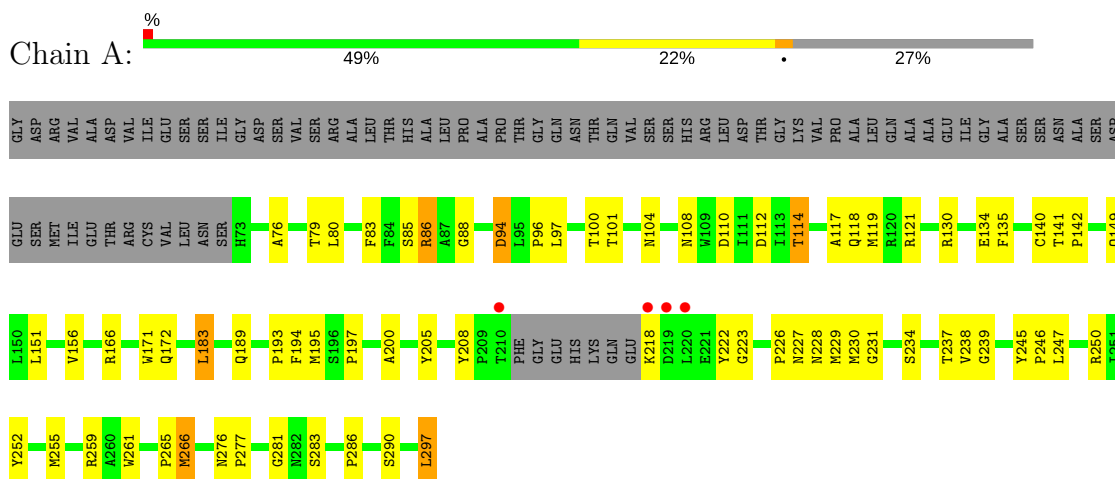
• Molecule 2: Genome Polyprotein, capsid protein VP2
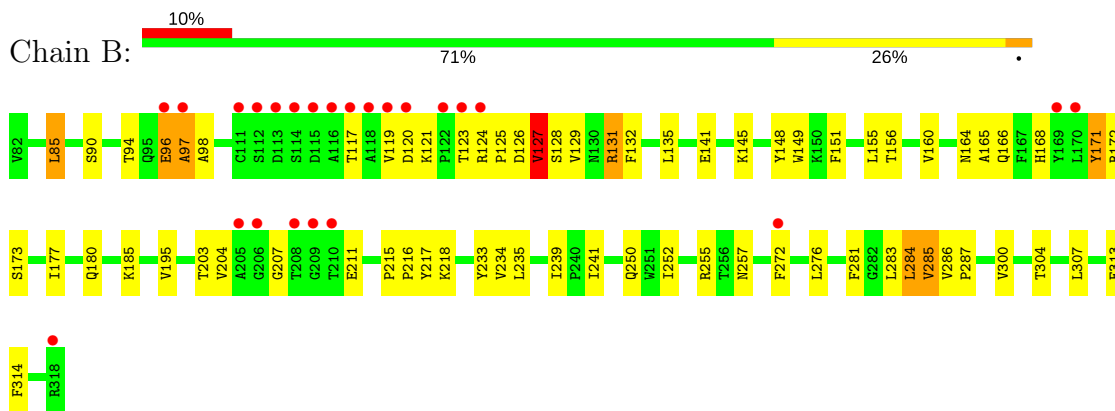
• Molecule 3: Genome Polyprotein, capsid protein VP3

V203 V204 P205 Y213 A218 A219 A220 Q221 M226 K227 L228 D234 I235 L236 Q237 T238 G239

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 42 3 2	Depositor
Cell constants a, b, c, α, β, γ	353.10Å 353.10Å 353.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.94 – 2.88 49.94 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.94-2.88) 99.4 (49.94-2.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.38	Depositor
$< I/\sigma(I) >$ [1]	1.06 (at 2.86Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.227 , 0.236 0.221 , 0.223	Depositor DCC
R_{free} test set	1666 reflections (1.01%)	DCC
Wilson B-factor (Å^2)	51.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 53.3	EDS
L-test for twinning[2]	$< |L| > = 0.45, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	5466	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.21% 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: NA

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	0/1776	0.74	0/2419
2	B	0.51	0/1889	0.74	0/2592
3	C	0.53	0/1891	0.78	1/2586 (0.0%)
All	All	0.51	0/5556	0.75	1/7597 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	192	GLY	N-CA-C	-5.05	100.47	113.10

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	63	0
2	B	1834	0	1774	55	0
3	C	1839	0	1814	73	0
4	A	1	0	0	0	0
5	A	20	0	0	1	0
5	B	23	0	0	2	0
5	C	25	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5466	0	5276	163	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 15.

All (163) 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)
3:C:58:VAL:HG23	3:C:59:PRO:HD3	1.37	1.03
1:A:281:GLY:HA3	2:B:204:VAL:HG13	1.45	0.98
1:A:229:MET:HE2	1:A:231:GLY:H	1.39	0.87
3:C:58:VAL:HG23	3:C:59:PRO:CD	2.08	0.83
3:C:105:CYS:HA	3:C:226:MET:HE2	1.60	0.82
2:B:233:TYR:HA	3:C:66:MET:HE3	1.61	0.82
2:B:250:GLN:HG3	5:B:419:HOH:O	1.80	0.81
2:B:218:LYS:HD2	2:B:218:LYS:H	1.45	0.79
1:A:140:CYS:HA	1:A:183:LEU:HD21	1.64	0.78
3:C:178:ARG:HH12	3:C:187:ASP:HB3	1.50	0.76
3:C:14:LEU:HD22	3:C:16:THR:H	1.50	0.76
1:A:297:LEU:H	1:A:297:LEU:HD12	1.51	0.75
1:A:130:ARG:NH2	3:C:31:THR:O	2.21	0.74
1:A:281:GLY:CA	2:B:204:VAL:HG13	2.16	0.74
3:C:178:ARG:HH12	3:C:187:ASP:CB	2.02	0.72
3:C:105:CYS:HA	3:C:226:MET:CE	2.20	0.72
1:A:104:ASN:O	1:A:166:ARG:HD2	1.90	0.72
3:C:66:MET:HE1	3:C:69:LEU:HD11	1.73	0.70
2:B:233:TYR:HA	3:C:66:MET:CE	2.21	0.70
2:B:85:LEU:HD21	2:B:94:THR:HG22	1.75	0.69
2:B:124:ARG:HG2	2:B:313:GLU:HG2	1.75	0.67
1:A:166:ARG:NH2	1:A:237:THR:OG1	2.27	0.67
1:A:114:THR:HG23	3:C:237:GLN:HG2	1.77	0.66
3:C:92:ARG:HD3	3:C:188:TYR:HD2	1.59	0.66
1:A:119:MET:SD	1:A:255:MET:HE1	2.36	0.66
2:B:204:VAL:HG12	2:B:207:GLY:H	1.60	0.66
1:A:141:THR:HB	1:A:142:PRO:HD2	1.79	0.64
2:B:85:LEU:HD21	2:B:94:THR:CG2	2.27	0.64
1:A:114:THR:HG21	3:C:237:GLN:HE21	1.63	0.64
2:B:218:LYS:N	2:B:218:LYS:HD2	2.12	0.63
2:B:195:VAL:HG13	2:B:281:PHE:CD2	2.33	0.63
3:C:91:GLY:HA3	3:C:111:TRP:CZ2	2.34	0.63
1:A:276:ASN:HB2	1:A:277:PRO:HD2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:PRO:HB3	2:B:129:VAL:HG21	1.81	0.62
1:A:261:TRP:CD1	3:C:36:ILE:HB	2.34	0.62
1:A:197:PRO:HA	3:C:31:THR:HG21	1.80	0.62
3:C:180:HIS:HE1	3:C:185:VAL:HG13	1.64	0.61
1:A:281:GLY:HA3	2:B:204:VAL:CG1	2.26	0.61
3:C:188:TYR:O	3:C:189:TYR:HB3	2.02	0.60
1:A:112:ASP:OD1	1:A:114:THR:HG22	2.02	0.59
1:A:208:TYR:CE1	1:A:222:TYR:HB2	2.39	0.58
1:A:117:ALA:HB1	3:C:236:LEU:HB3	1.86	0.58
2:B:203:THR:HG23	2:B:215:PRO:HG3	1.85	0.58
3:C:65:LEU:O	3:C:68:ARG:HG3	2.05	0.57
2:B:148:TYR:HB3	2:B:284:LEU:CD1	2.35	0.56
2:B:128:SER:O	2:B:131:ARG:HG2	2.05	0.56
3:C:9:GLY:O	3:C:12:GLN:HG2	2.05	0.56
1:A:134:GLU:HG3	3:C:21:SER:OG	2.06	0.56
1:A:226:PRO:C	1:A:228:ASN:H	2.09	0.56
2:B:180:GLN:HB3	5:B:415:HOH:O	2.07	0.55
2:B:123:THR:O	2:B:125:PRO:HD3	2.07	0.55
3:C:180:HIS:CD2	3:C:181:ALA:H	2.25	0.55
3:C:73:VAL:HA	3:C:198:TYR:OH	2.07	0.55
3:C:130:LYS:HB2	3:C:200:THR:HG23	1.87	0.55
2:B:149:TRP:HZ3	2:B:285:VAL:HG13	1.71	0.54
1:A:205:TYR:O	1:A:223:GLY:HA2	2.08	0.54
1:A:250:ARG:HH21	1:A:250:ARG:HG3	1.73	0.54
3:C:56:ASN:OD1	3:C:58:VAL:HG22	2.08	0.54
3:C:178:ARG:HG2	3:C:179:ALA:N	2.23	0.53
1:A:238:VAL:HG12	1:A:239:GLY:N	2.22	0.53
2:B:148:TYR:HA	2:B:283:LEU:O	2.09	0.53
3:C:115:LEU:HB2	3:C:169:ILE:HB	1.90	0.53
3:C:204:VAL:HG22	3:C:205:PRO:HD2	1.91	0.53
2:B:155:LEU:HD21	2:B:307:LEU:HD11	1.90	0.53
3:C:44:LEU:O	3:C:48:GLN:HG3	2.09	0.53
3:C:132:LEU:C	3:C:132:LEU:HD23	2.30	0.52
3:C:174:ASN:O	3:C:174:ASN:OD1	2.27	0.52
1:A:290:SER:OG	3:C:68:ARG:NH2	2.42	0.52
3:C:85:VAL:HG21	3:C:142:LEU:HD12	1.91	0.52
2:B:156:THR:HG22	2:B:165:ALA:HB1	1.93	0.51
3:C:109:THR:HB	3:C:228:LEU:HB3	1.91	0.51
1:A:151:LEU:HD11	1:A:183:LEU:HD12	1.91	0.51
1:A:121:ARG:CZ	1:A:266:MET:HE3	2.41	0.51
5:A:401:HOH:O	3:C:31:THR:HG23	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:TYR:CE2	2:B:173:SER:HB3	2.47	0.50
1:A:229:MET:HE2	1:A:231:GLY:N	2.19	0.50
3:C:58:VAL:CG2	3:C:59:PRO:CD	2.86	0.50
3:C:178:ARG:HD3	3:C:180:HIS:HB3	1.93	0.50
2:B:117:THR:CG2	2:B:120:ASP:HB3	2.42	0.50
1:A:194:PHE:CZ	1:A:200:ALA:HA	2.47	0.49
2:B:96:GLU:O	2:B:97:ALA:HB2	2.12	0.49
1:A:112:ASP:OD2	1:A:114:THR:HB	2.12	0.49
1:A:229:MET:HE2	1:A:230:MET:H	1.78	0.49
2:B:235:LEU:HD21	2:B:241:ILE:HG13	1.94	0.48
3:C:92:ARG:HD2	3:C:187:ASP:OD1	2.11	0.48
1:A:149:GLN:HG2	1:A:247:LEU:HD11	1.94	0.48
2:B:126:ASP:O	2:B:127:VAL:C	2.51	0.48
3:C:180:HIS:CG	3:C:181:ALA:H	2.32	0.48
1:A:156:VAL:HG22	1:A:156:VAL:O	2.14	0.48
1:A:76:ALA:O	1:A:79:THR:HG23	2.13	0.47
3:C:234:ASP:O	3:C:236:LEU:HD12	2.14	0.47
1:A:86:ARG:HG2	3:C:16:THR:HG22	1.96	0.47
3:C:2:PHE:CD1	3:C:3:PRO:HD2	2.49	0.47
1:A:218:LYS:N	2:B:217:TYR:H	2.12	0.47
3:C:142:LEU:HD23	3:C:143:PRO:O	2.14	0.47
3:C:50:GLU:HA	3:C:219:ALA:HB2	1.96	0.47
2:B:168:HIS:CD2	2:B:314:PHE:HB3	2.49	0.47
3:C:188:TYR:O	3:C:189:TYR:HD2	1.98	0.47
1:A:229:MET:HE2	1:A:230:MET:N	2.30	0.47
3:C:66:MET:HE1	3:C:69:LEU:CD1	2.42	0.47
1:A:226:PRO:O	1:A:228:ASN:N	2.44	0.46
2:B:151:PHE:CE2	2:B:307:LEU:HD22	2.51	0.46
2:B:185:LYS:HD3	3:C:125:PHE:CD1	2.51	0.45
2:B:121:LYS:HG2	2:B:121:LYS:H	1.56	0.45
2:B:252:ILE:HA	2:B:257:ASN:HD21	1.82	0.45
2:B:185:LYS:HD3	3:C:125:PHE:CE1	2.52	0.45
1:A:114:THR:HG23	1:A:114:THR:O	2.15	0.45
2:B:172:ARG:HD2	2:B:272:PHE:CZ	2.52	0.45
1:A:135:PHE:O	1:A:189:GLN:HA	2.17	0.45
3:C:72:PRO:HB3	3:C:213:TYR:CE2	2.51	0.45
2:B:155:LEU:HD11	2:B:307:LEU:CD1	2.46	0.44
3:C:109:THR:HB	3:C:228:LEU:CB	2.48	0.44
1:A:193:PRO:HG2	1:A:195:MET:SD	2.57	0.44
2:B:141:GLU:HG2	2:B:300:VAL:HG12	2.00	0.44
2:B:203:THR:HG23	2:B:215:PRO:CG	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:188:TYR:O	3:C:189:TYR:CB	2.66	0.44
1:A:238:VAL:CG1	1:A:239:GLY:N	2.81	0.43
2:B:168:HIS:CG	2:B:314:PHE:HB3	2.53	0.43
1:A:229:MET:CE	1:A:230:MET:H	2.32	0.43
2:B:90:SER:HB2	2:B:132:PHE:HB2	2.01	0.43
1:A:286:PRO:HB2	3:C:68:ARG:NH1	2.33	0.43
2:B:203:THR:HG23	2:B:215:PRO:CD	2.48	0.43
1:A:171:TRP:CH2	1:A:234:SER:HB3	2.54	0.43
1:A:208:TYR:HE1	1:A:222:TYR:HB2	1.83	0.43
1:A:281:GLY:N	2:B:204:VAL:HG13	2.32	0.43
1:A:83:PHE:CD1	3:C:43:LEU:HD11	2.54	0.43
3:C:91:GLY:HA3	3:C:111:TRP:HZ2	1.80	0.43
1:A:97:LEU:HD11	1:A:246:PRO:HD3	2.01	0.43
1:A:265:PRO:HB2	2:B:239:ILE:HB	2.00	0.42
1:A:297:LEU:H	1:A:297:LEU:CD1	2.18	0.42
1:A:114:THR:CG2	3:C:237:GLN:HG2	2.47	0.42
3:C:50:GLU:HA	3:C:218:ALA:O	2.18	0.42
3:C:4:THR:HG22	3:C:5:GLU:N	2.33	0.42
1:A:261:TRP:CD1	3:C:39:GLU:HB2	2.53	0.42
3:C:61:ASN:ND2	3:C:64:SER:OG	2.52	0.42
1:A:218:LYS:N	2:B:217:TYR:N	2.66	0.42
3:C:75:ALA:HA	3:C:202:TYR:HB3	2.01	0.42
2:B:172:ARG:HD3	2:B:313:GLU:OE2	2.20	0.42
2:B:215:PRO:HA	2:B:216:PRO:HD3	1.80	0.42
1:A:108:ASN:ND2	1:A:234:SER:OG	2.52	0.41
3:C:221:GLN:HG3	5:C:308:HOH:O	2.19	0.41
1:A:259:ARG:NH1	3:C:39:GLU:OE1	2.53	0.41
3:C:105:CYS:SG	3:C:226:MET:CE	3.08	0.41
3:C:29:HIS:HA	3:C:30:PRO:HD2	1.86	0.41
2:B:233:TYR:CA	3:C:66:MET:CE	2.97	0.41
1:A:156:VAL:CG2	1:A:156:VAL:O	2.67	0.41
1:A:94:ASP:C	1:A:96:PRO:HD3	2.41	0.41
2:B:148:TYR:HB3	2:B:284:LEU:HD12	2.03	0.41
2:B:164:ASN:O	2:B:168:HIS:HB2	2.20	0.41
2:B:234:VAL:HA	2:B:239:ILE:O	2.21	0.41
2:B:177:ILE:HG21	2:B:283:LEU:HD22	2.03	0.41
3:C:14:LEU:HB3	3:C:17:ASP:HB2	2.03	0.41
3:C:58:VAL:H	3:C:59:PRO:HD2	1.85	0.41
1:A:117:ALA:HB1	3:C:236:LEU:HD23	2.03	0.41
3:C:42:ASN:O	3:C:45:GLU:HG3	2.21	0.41
1:A:88:GLY:O	1:A:252:TYR:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:286:VAL:HA	2:B:287:PRO:HD3	1.89	0.41
1:A:121:ARG:NH1	1:A:266:MET:HE3	2.36	0.40
2:B:166:GLN:HG2	2:B:276:LEU:HD21	2.03	0.40
1:A:108:ASN:HA	1:A:108:ASN:HD22	1.67	0.40
1:A:118:GLN:H	1:A:118:GLN:HG2	1.54	0.40
2:B:255:ARG:NH2	3:C:124:SER:O	2.55	0.40
3:C:188:TYR:O	3:C:189:TYR:CD2	2.75	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	214/297 (72%)	201 (94%)	10 (5%)	3 (1%)	13	40
2	B	235/237 (99%)	221 (94%)	10 (4%)	4 (2%)	11	34
3	C	237/239 (99%)	216 (91%)	14 (6%)	7 (3%)	5	19
All	All	686/773 (89%)	638 (93%)	34 (5%)	14 (2%)	9	30

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	96	GLU
2	B	127	VAL
3	C	180	HIS
3	C	188	TYR
1	A	227	ASN
2	B	97	ALA
2	B	98	ALA
3	C	181	ALA
3	C	189	TYR
1	A	85	SER

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Mol	Chain	Res	Type
1	A	86	ARG
3	C	58	VAL
3	C	182	ARG
3	C	228	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	187/251 (74%)	175 (94%)	12 (6%)	20	48
2	B	201/201 (100%)	189 (94%)	12 (6%)	22	52
3	C	199/199 (100%)	181 (91%)	18 (9%)	11	30
All	All	587/651 (90%)	545 (93%)	42 (7%)	17	42

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	LEU
1	A	94	ASP
1	A	100	THR
1	A	101	THR
1	A	110	ASP
1	A	114	THR
1	A	172	GLN
1	A	183	LEU
1	A	245	TYR
1	A	266	MET
1	A	283	SER
1	A	297	LEU
2	B	85	LEU
2	B	119	VAL
2	B	127	VAL
2	B	131	ARG
2	B	135	LEU
2	B	145	LYS

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Mol	Chain	Res	Type
2	B	160	VAL
2	B	171	TYR
2	B	211	GLU
2	B	284	LEU
2	B	285	VAL
2	B	304	THR
3	C	14	LEU
3	C	20	VAL
3	C	25	LEU
3	C	33	CYS
3	C	53	LEU
3	C	70	ARG
3	C	72	PRO
3	C	87	ARG
3	C	90	PRO
3	C	116	GLU
3	C	136	THR
3	C	141	PRO
3	C	146	ARG
3	C	186	PHE
3	C	204	VAL
3	C	228	LEU
3	C	234	ASP
3	C	236	LEU

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	227	ASN
1	A	228	ASN
2	B	168	HIS
2	B	188	GLN
2	B	214	HIS
2	B	277	ASN
3	C	11	ASN
3	C	61	ASN
3	C	93	ASN
3	C	174	ASN
3	C	180	HIS
3	C	210	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 ⓘ

Of 1 ligands modelled in this entry, 1 is 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 (i)

6.1   Protein, DNA and RNA chains (i)

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	218/297 (73%)	-0.35	4 (1%) 69	67	32, 50, 103, 161	0
2	B	237/237 (100%)	0.13	24 (10%) 8	5	34, 64, 147, 190	0
3	C	239/239 (100%)	-0.24	12 (5%) 30	26	33, 52, 133, 186	0
All	All	694/773 (89%)	-0.15	40 (5%) 24	19	32, 54, 133, 190	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	114	SER	7.7
2	B	115	ASP	7.4
1	A	218	LYS	7.2
3	C	180	HIS	7.1
3	C	183	ASP	7.1
3	C	177	TYR	6.8
3	C	182	ARG	6.7
3	C	181	ALA	6.5
2	B	120	ASP	6.0
2	B	113	ASP	5.9
3	C	176	HIS	5.3
2	B	117	THR	4.7
2	B	116	ALA	4.3
2	B	118	ALA	4.0
3	C	184	GLY	4.0
2	B	111	CYS	3.9
3	C	189	TYR	3.9
1	A	219	ASP	3.8
3	C	178	ARG	3.6
1	A	220	LEU	3.6
3	C	190	THR	3.5
2	B	119	VAL	3.4
2	B	96	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	209	GLY	3.3
3	C	186	PHE	3.0
2	B	210	THR	3.0
2	B	112	SER	2.8
2	B	169	TYR	2.8
2	B	318	ARG	2.8
2	B	124	ARG	2.8
2	B	123	THR	2.8
1	A	210	THR	2.8
2	B	122	PRO	2.7
2	B	208	THR	2.5
2	B	205	ALA	2.3
3	C	185	VAL	2.2
2	B	206	GLY	2.1
2	B	272	PHE	2.1
2	B	97	ALA	2.1
2	B	170	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 ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
4	NA	A	301	1/1	0.80	0.20	-	56,56,56,56	0

6.5 Other polymers ⓘ

There are no such residues in this entry.