



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:47 PM UTC

PDB ID : 8ZHW / pdb_00008zhw
Title : Structure of Mokola lyssavirus glycoprotein in post-fusion state
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Deposited on : 2024-05-11
Resolution : 3.20 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

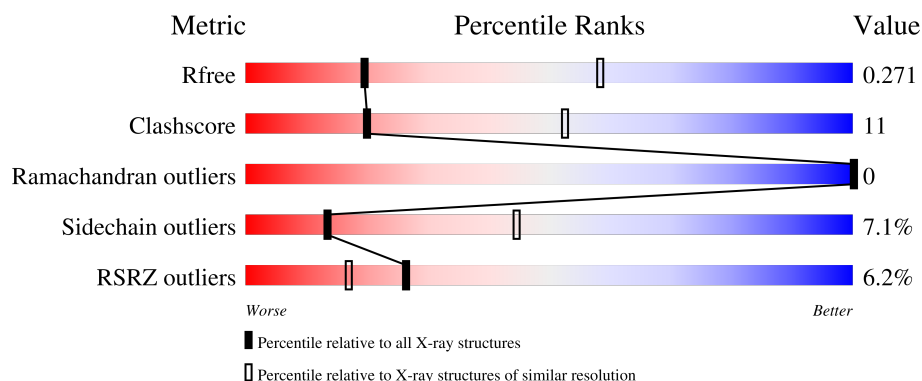
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 $\leq 5\%$. 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	436	
1	B	436	
1	C	436	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7217 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 Glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2663	1699	454	487	23			
1	B	285	Total	C	N	O	S	0	0	0
			2275	1456	387	413	19			
1	C	286	Total	C	N	O	S	0	0	0
			2279	1452	388	419	20			

There are 48 discrepancies between the modelled and reference sequences:

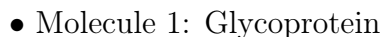
Chain	Residue	Modelled	Actual	Comment	Reference
A	75	GLY	-	linker	UNP P0C572
A	76	GLY	-	linker	UNP P0C572
A	77	SER	-	linker	UNP P0C572
A	78	GLY	-	linker	UNP P0C572
A	79	GLY	-	linker	UNP P0C572
A	121	GLY	-	linker	UNP P0C572
A	122	GLY	-	linker	UNP P0C572
A	123	SER	-	linker	UNP P0C572
A	124	GLY	-	linker	UNP P0C572
A	125	GLY	-	linker	UNP P0C572
A	437	HIS	-	expression tag	UNP P0C572
A	438	HIS	-	expression tag	UNP P0C572
A	439	HIS	-	expression tag	UNP P0C572
A	440	HIS	-	expression tag	UNP P0C572
A	441	HIS	-	expression tag	UNP P0C572
A	442	HIS	-	expression tag	UNP P0C572
B	79	GLY	-	linker	UNP P0C572
B	80	GLY	-	linker	UNP P0C572
B	81	SER	-	linker	UNP P0C572
B	82	GLY	-	linker	UNP P0C572
B	83	GLY	-	linker	UNP P0C572
B	121	GLY	-	linker	UNP P0C572
B	122	GLY	-	linker	UNP P0C572

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Chain	Residue	Modelled	Actual	Comment	Reference
B	123	SER	-	linker	UNP P0C572
B	124	GLY	-	linker	UNP P0C572
B	125	GLY	-	linker	UNP P0C572
B	437	HIS	-	expression tag	UNP P0C572
B	438	HIS	-	expression tag	UNP P0C572
B	439	HIS	-	expression tag	UNP P0C572
B	440	HIS	-	expression tag	UNP P0C572
B	441	HIS	-	expression tag	UNP P0C572
B	442	HIS	-	expression tag	UNP P0C572
C	79	GLY	-	linker	UNP P0C572
C	80	GLY	-	linker	UNP P0C572
C	81	SER	-	linker	UNP P0C572
C	82	GLY	-	linker	UNP P0C572
C	83	GLY	-	linker	UNP P0C572
C	121	GLY	-	linker	UNP P0C572
C	122	GLY	-	linker	UNP P0C572
C	123	SER	-	linker	UNP P0C572
C	124	GLY	-	linker	UNP P0C572
C	125	GLY	-	linker	UNP P0C572
C	437	HIS	-	expression tag	UNP P0C572
C	438	HIS	-	expression tag	UNP P0C572
C	439	HIS	-	expression tag	UNP P0C572
C	440	HIS	-	expression tag	UNP P0C572
C	441	HIS	-	expression tag	UNP P0C572
C	442	HIS	-	expression tag	UNP P0C572

- Molecule 1: Glycoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	104.23Å 87.52Å 111.19Å 90.00° 111.87° 90.00°	Depositor
Resolution (Å)	48.37 – 3.20 48.37 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.0 (48.37-3.20) 95.0 (48.37-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.246 , 0.288 (Not available) , 0.271	Depositor DCC
R_{free} test set	1429 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	107.2	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 78.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7217	wwPDB-VP
Average B, all atoms (Å ²)	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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 [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.23	0/2720	0.48	2/3669 (0.1%)
1	B	0.21	0/2325	0.45	0/3132
1	C	0.19	0/2326	0.45	0/3133
All	All	0.21	0/7371	0.46	2/9934 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	CYS	N-CA-C	8.36	128.60	110.80
1	A	252	CYS	CB-CA-C	-5.38	99.70	110.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2663	0	2639	77	0
1	B	2275	0	2278	40	0
1	C	2279	0	2268	49	0
All	All	7217	0	7185	164	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 11.

All (164) 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:340:PRO:HG2	1:A:346:LYS:HZ1	1.36	0.89
1:A:339:LEU:H	1:A:339:LEU:HD12	1.40	0.87
1:A:340:PRO:HG2	1:A:346:LYS:NZ	1.91	0.85
1:C:339:LEU:HB2	1:C:372:LEU:HD22	1.63	0.80
1:B:1:GLU:HG3	1:B:331:ARG:HH12	1.47	0.79
1:A:371:ILE:HG22	1:A:372:LEU:HG	1.66	0.76
1:C:1:GLU:HG3	1:C:331:ARG:HH12	1.51	0.75
1:A:260:ILE:HG23	1:A:395:LEU:HD11	1.68	0.74
1:A:56:VAL:HG22	1:A:188:VAL:HG11	1.70	0.73
1:C:19:MET:HE1	1:C:294:GLN:HA	1.71	0.73
1:C:41:PHE:HE1	1:C:43:TYR:HB3	1.56	0.70
1:A:339:LEU:HD12	1:A:339:LEU:N	2.03	0.70
1:A:341:SER:O	1:A:342:LYS:C	2.32	0.69
1:B:338:ILE:HG13	1:B:339:LEU:HD23	1.73	0.69
1:A:1:GLU:HG3	1:A:331:ARG:HH12	1.58	0.69
1:A:226:THR:HG22	1:A:231:PRO:HA	1.76	0.68
1:A:338:ILE:HG13	1:A:339:LEU:HG	1.76	0.68
1:A:345:LEU:HB2	1:A:372:LEU:HD22	1.75	0.67
1:A:25:PRO:O	1:A:26:ASN:ND2	2.16	0.67
1:A:337:ASP:N	1:A:337:ASP:OD1	2.27	0.67
1:C:6:THR:OG1	1:C:306:LYS:O	2.13	0.66
1:C:331:ARG:NH2	1:C:333:ASP:OD2	2.28	0.66
1:A:366:GLY:HA3	1:A:370:GLN:HB2	1.78	0.66
1:C:357:GLY:HA2	1:C:365:LYS:HB2	1.78	0.65
1:A:141:GLU:HB3	1:A:150:HIS:HB2	1.79	0.64
1:C:47:LYS:HG2	1:C:193:THR:HG23	1.77	0.64
1:A:298:PHE:HA	1:A:301:LEU:HD23	1.79	0.63
1:B:313:LYS:NZ	1:B:326:ASN:OD1	2.25	0.62
1:A:17:ILE:HD12	1:A:21:HIS:HB3	1.82	0.62
1:B:240:TRP:HB2	1:B:258:ILE:HG21	1.82	0.61
1:C:51:LEU:HD21	1:C:191:ILE:HB	1.83	0.61
1:A:62:THR:HB	1:A:133:LEU:HB3	1.82	0.60
1:C:2:PHE:HB2	1:C:385:MET:HE1	1.84	0.60
1:B:223:CYS:SG	1:B:234:ARG:HB3	2.41	0.60
1:B:41:PHE:HE1	1:B:43:TYR:HB3	1.65	0.59
1:A:252:CYS:O	1:A:253:THR:C	2.43	0.59
1:B:4:LEU:HD13	1:B:382:LYS:HD3	1.84	0.59
1:B:382:LYS:NZ	1:B:386:ASP:OD1	2.35	0.59
1:A:227:LEU:HD11	1:A:258:ILE:HG12	1.85	0.59
1:C:298:PHE:HA	1:C:301:LEU:HD23	1.85	0.59
1:A:16:PRO:HG3	1:A:323:MET:HE2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:LYS:HB3	1:A:371:ILE:HD13	1.86	0.58
1:B:226:THR:HG22	1:B:231:PRO:HA	1.84	0.58
1:C:357:GLY:H	1:C:365:LYS:HE2	1.68	0.58
1:C:26:ASN:ND2	1:C:31:GLU:OE2	2.36	0.57
1:A:19:MET:HE1	1:A:294:GLN:HA	1.86	0.57
1:A:298:PHE:O	1:A:301:LEU:HB2	2.05	0.57
1:A:375:GLU:N	1:A:375:GLU:OE1	2.38	0.57
1:C:226:THR:HG22	1:C:231:PRO:HA	1.86	0.56
1:B:354:PRO:HB3	1:B:359:LEU:HG	1.87	0.56
1:A:260:ILE:HD11	1:A:393:PHE:HD2	1.68	0.56
1:C:26:ASN:ND2	1:C:26:ASN:O	2.39	0.56
1:B:26:ASN:O	1:B:26:ASN:ND2	2.39	0.56
1:A:335:TRP:O	1:A:339:LEU:HD11	2.06	0.56
1:B:47:LYS:HE2	1:B:191:ILE:HA	1.87	0.56
1:B:268:ILE:HD13	1:B:387:LEU:HB3	1.87	0.56
1:B:16:PRO:HG3	1:B:323:MET:HE2	1.89	0.55
1:B:30:SER:OG	1:B:35:CYS:O	2.23	0.55
1:B:47:LYS:HG2	1:B:193:THR:HG23	1.87	0.55
1:A:32:GLU:OE2	1:A:306:LYS:NZ	2.26	0.55
1:A:354:PRO:HB3	1:A:359:LEU:HG	1.87	0.55
1:A:335:TRP:O	1:A:339:LEU:CD1	2.55	0.55
1:A:62:THR:HG23	1:A:176:THR:HG22	1.89	0.54
1:B:27:ASN:ND2	1:B:307:LEU:H	2.05	0.54
1:B:298:PHE:HA	1:B:301:LEU:HD23	1.89	0.54
1:C:4:LEU:HD13	1:C:382:LYS:HD3	1.90	0.54
1:A:343:GLY:HA2	1:A:371:ILE:HG23	1.90	0.53
1:B:313:LYS:O	1:B:329:TYR:OH	2.21	0.53
1:B:213:ARG:NH2	1:B:266:ASP:OD1	2.41	0.53
1:A:8:PRO:HG2	1:A:360:PHE:HE2	1.74	0.53
1:A:162:VAL:H	1:C:380:GLN:HE22	1.56	0.53
1:C:354:PRO:HB3	1:C:359:LEU:HG	1.89	0.52
1:A:223:CYS:SG	1:A:234:ARG:HB3	2.50	0.52
1:C:370:GLN:HB3	1:C:372:LEU:HD12	1.92	0.52
1:B:272:ILE:HG23	1:B:381:LEU:HD11	1.92	0.52
1:A:18:ASP:OD1	1:A:19:MET:N	2.43	0.52
1:C:1:GLU:HG3	1:C:331:ARG:NH1	2.22	0.51
1:A:370:GLN:C	1:A:371:ILE:HG13	2.34	0.51
1:A:314:ALA:O	1:A:324:GLU:HA	2.11	0.51
1:A:343:GLY:HA2	1:A:371:ILE:CG2	2.41	0.51
1:C:344:CYS:O	1:C:372:LEU:HD23	2.10	0.51
1:B:39:SER:O	1:B:198:LYS:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ARG:N	1:B:213:ARG:HE	2.09	0.51
1:C:223:CYS:SG	1:C:234:ARG:HB3	2.51	0.50
1:A:367:PRO:HD2	1:A:370:GLN:OE1	2.11	0.50
1:A:37:ALA:HB3	1:A:201:MET:O	2.11	0.50
1:A:1:GLU:O	1:A:331:ARG:NH1	2.42	0.50
1:A:138:SER:OG	1:A:178:TRP:NE1	2.45	0.50
1:A:41:PHE:CE2	1:A:43:TYR:HB3	2.47	0.49
1:C:18:ASP:OD1	1:C:20:ILE:HG22	2.12	0.49
1:A:340:PRO:CG	1:A:346:LYS:NZ	2.69	0.49
1:C:27:ASN:HD22	1:C:307:LEU:H	1.59	0.49
1:A:260:ILE:HD11	1:A:393:PHE:CD2	2.48	0.48
1:B:217:ARG:NE	1:B:237:ASP:OD2	2.44	0.48
1:C:159:CYS:SG	1:C:160:SER:N	2.86	0.48
1:C:265:LEU:O	1:C:269:GLU:HG3	2.13	0.47
1:A:41:PHE:HE2	1:A:43:TYR:HB3	1.78	0.47
1:A:265:LEU:HD12	1:A:388:LEU:HD11	1.96	0.47
1:B:13:LYS:N	1:B:13:LYS:HD3	2.30	0.47
1:B:45:GLU:OE2	1:B:213:ARG:NH1	2.48	0.47
1:B:265:LEU:O	1:B:269:GLU:HG3	2.14	0.47
1:A:47:LYS:HD3	1:A:193:THR:HG23	1.97	0.47
1:B:143:ASP:OD1	1:B:398:PRO:HD2	2.15	0.47
1:C:379:GLU:O	1:C:383:GLN:HB2	2.15	0.47
1:A:374:PRO:HD2	1:A:376:MET:HE3	1.97	0.46
1:B:1:GLU:O	1:B:331:ARG:NH1	2.48	0.46
1:B:38:GLU:HA	1:B:199:LYS:O	2.15	0.46
1:C:213:ARG:HE	1:C:213:ARG:HB3	1.62	0.46
1:A:162:VAL:H	1:C:380:GLN:NE2	2.13	0.46
1:A:44:PHE:O	1:A:241:VAL:HA	2.15	0.46
1:C:264:ARG:HD2	1:C:268:ILE:HD11	1.98	0.46
1:C:370:GLN:HB3	1:C:372:LEU:CD1	2.46	0.46
1:A:30:SER:OG	1:A:35:CYS:O	2.27	0.45
1:A:366:GLY:HA3	1:A:370:GLN:CB	2.45	0.45
1:C:37:ALA:HB3	1:C:201:MET:O	2.15	0.45
1:A:223:CYS:HA	1:A:250:VAL:HG23	1.97	0.45
1:A:58:GLY:HA3	1:A:178:TRP:CZ2	2.52	0.45
1:B:342:LYS:O	1:B:372:LEU:HD21	2.16	0.45
1:B:330:LYS:HA	1:B:330:LYS:HD2	1.69	0.45
1:C:210:LYS:HG3	1:C:216:TYR:HD1	1.82	0.45
1:C:286:THR:HG23	1:C:300:ARG:HG3	1.99	0.45
1:C:47:LYS:HB2	1:C:51:LEU:HD22	1.99	0.45
1:A:142:MET:HA	1:A:148:THR:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:ALA:O	1:B:200:ALA:HA	2.18	0.44
1:C:354:PRO:HG2	1:C:365:LYS:HD3	2.00	0.44
1:A:371:ILE:HG22	1:A:372:LEU:N	2.33	0.44
1:B:28:LEU:HB2	1:B:31:GLU:HG2	2.00	0.44
1:C:260:ILE:HD11	1:C:393:PHE:HD2	1.82	0.44
1:C:217:ARG:NE	1:C:237:ASP:OD2	2.44	0.44
1:B:18:ASP:OD1	1:B:20:ILE:HG22	2.17	0.43
1:C:240:TRP:HB2	1:C:258:ILE:HG21	1.99	0.43
1:C:337:ASP:N	1:C:337:ASP:OD1	2.52	0.43
1:A:232:GLY:HA3	1:A:240:TRP:CZ2	2.54	0.43
1:B:393:PHE:HA	1:B:394:PRO:HD3	1.87	0.43
1:A:255:ASN:N	1:A:255:ASN:OD1	2.52	0.43
1:B:271:LEU:HD23	1:B:384:HIS:NE2	2.33	0.43
1:A:228:CYS:SG	1:A:228:CYS:O	2.77	0.43
1:B:328:TYR:HD1	1:B:329:TYR:N	2.17	0.43
1:C:354:PRO:CG	1:C:365:LYS:HD3	2.49	0.43
1:A:268:ILE:HD13	1:A:387:LEU:HB3	2.01	0.42
1:C:342:LYS:NZ	1:C:369:GLY:HA2	2.33	0.42
1:C:375:GLU:OE1	1:C:375:GLU:N	2.52	0.42
1:A:371:ILE:HG22	1:A:372:LEU:H	1.84	0.42
1:A:271:LEU:HD23	1:A:384:HIS:CD2	2.54	0.42
1:A:298:PHE:CZ	1:A:358:VAL:HG13	2.54	0.42
1:C:238:GLY:O	1:C:258:ILE:HA	2.20	0.42
1:C:16:PRO:HG3	1:C:323:MET:HE2	2.02	0.42
1:B:217:ARG:HE	1:B:237:ASP:CG	2.28	0.41
1:C:341:SER:HB2	1:C:344:CYS:HB2	2.02	0.41
1:A:47:LYS:HG2	1:A:191:ILE:C	2.45	0.41
1:C:342:LYS:O	1:C:370:GLN:HA	2.19	0.41
1:C:334:LYS:HB2	1:C:334:LYS:HE3	1.85	0.41
1:A:258:ILE:H	1:A:258:ILE:HG13	1.72	0.41
1:A:205:ARG:NH2	1:A:207:CYS:SG	2.94	0.41
1:A:301:LEU:HD13	1:A:301:LEU:HA	1.84	0.41
1:A:56:VAL:HB	1:A:140:VAL:HG23	2.03	0.41
1:A:289:THR:HA	1:A:292:MET:HE2	2.02	0.41
1:A:368:ASP:O	1:A:370:GLN:HG3	2.20	0.41
1:A:372:LEU:HG	1:A:372:LEU:H	1.55	0.41
1:B:56:VAL:HB	1:B:141:GLU:N	2.35	0.41
1:C:232:GLY:HA3	1:C:240:TRP:CZ2	2.56	0.41
1:A:17:ILE:HG21	1:A:324:GLU:HG2	2.03	0.40
1:A:14:TRP:CE3	1:A:14:TRP:HA	2.57	0.40
1:A:26:ASN:HB2	1:A:280:ARG:CZ	2.51	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	328/436 (75%)	301 (92%)	27 (8%)	0	100	100
1	B	277/436 (64%)	256 (92%)	21 (8%)	0	100	100
1	C	276/436 (63%)	261 (95%)	15 (5%)	0	100	100
All	All	881/1308 (67%)	818 (93%)	63 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	299/388 (77%)	266 (89%)	33 (11%)	6	26
1	B	257/388 (66%)	244 (95%)	13 (5%)	21	54
1	C	258/388 (66%)	246 (95%)	12 (5%)	23	57
All	All	814/1164 (70%)	756 (93%)	58 (7%)	13	44

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	10	LYS

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Mol	Chain	Res	Type
1	A	11	ILE
1	A	26	ASN
1	A	27	ASN
1	A	45	GLU
1	A	46	LEU
1	A	51	LEU
1	A	55	LYS
1	A	57	PRO
1	A	102	VAL
1	A	139	ILE
1	A	167	PRO
1	A	184	SER
1	A	187	LEU
1	A	189	CYS
1	A	193	THR
1	A	213	ARG
1	A	244	THR
1	A	250	VAL
1	A	252	CYS
1	A	260	ILE
1	A	274	GLU
1	A	296	VAL
1	A	301	LEU
1	A	327	VAL
1	A	337	ASP
1	A	339	LEU
1	A	344	CYS
1	A	345	LEU
1	A	346	LYS
1	A	358	VAL
1	A	372	LEU
1	B	13	LYS
1	B	57	PRO
1	B	228	CYS
1	B	252	CYS
1	B	265	LEU
1	B	296	VAL
1	B	324	GLU
1	B	339	LEU
1	B	344	CYS
1	B	364	ILE
1	B	372	LEU

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Mol	Chain	Res	Type
1	B	375	GLU
1	B	397	HIS
1	C	13	LYS
1	C	27	ASN
1	C	50	TYR
1	C	213	ARG
1	C	228	CYS
1	C	252	CYS
1	C	296	VAL
1	C	339	LEU
1	C	344	CYS
1	C	364	ILE
1	C	372	LEU
1	C	397	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	ASN
1	A	294	GLN
1	A	326	ASN
1	B	27	ASN
1	B	36	ASN
1	B	361	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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	338/436 (77%)	0.34	17 (5%) 34 22	85, 125, 204, 261	0
1	B	285/436 (65%)	0.42	24 (8%) 17 11	96, 136, 199, 232	0
1	C	286/436 (65%)	0.46	15 (5%) 33 21	81, 130, 201, 271	0
All	All	909/1308 (69%)	0.40	56 (6%) 26 17	81, 130, 203, 271	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	162	VAL	4.6
1	A	50	TYR	4.5
1	A	167	PRO	4.4
1	C	300	ARG	4.3
1	B	341	SER	4.2
1	B	366	GLY	4.0
1	B	396	ARG	3.9
1	B	185	LEU	3.7
1	C	254	PRO	3.7
1	C	284	LEU	3.4
1	B	373	ILE	3.3
1	A	184	SER	3.3
1	C	288	GLU	3.2
1	A	400	ILE	3.1
1	A	329	TYR	3.0
1	C	149	LEU	3.0
1	A	377	GLN	3.0
1	C	282	GLU	2.9
1	C	50	TYR	2.8
1	C	381	LEU	2.7
1	B	344	CYS	2.7
1	A	63	GLY	2.7
1	B	194	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	36	ASN	2.7
1	B	56	VAL	2.6
1	C	303	HIS	2.5
1	B	319	ASN	2.5
1	B	8	PRO	2.5
1	A	299	ARG	2.4
1	A	96	ASP	2.4
1	C	215	PHE	2.4
1	A	308	VAL	2.4
1	B	57	PRO	2.4
1	B	355	VAL	2.3
1	B	35	CYS	2.3
1	A	247	ASP	2.3
1	C	374	PRO	2.3
1	B	184	SER	2.3
1	B	266	ASP	2.3
1	B	372	LEU	2.2
1	C	53	HIS	2.2
1	A	307	LEU	2.2
1	A	403	GLU	2.2
1	B	1	GLU	2.2
1	A	29	LEU	2.1
1	A	359	LEU	2.1
1	C	287	LEU	2.1
1	C	22	LEU	2.1
1	B	299	ARG	2.1
1	B	398	PRO	2.1
1	B	263	ASP	2.1
1	A	93	ALA	2.1
1	B	333	ASP	2.0
1	B	142	MET	2.0
1	B	397	HIS	2.0
1	C	285	ASP	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 oligosaccharides 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.