



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:43 AM UTC

PDB ID : 6N9N / pdb_00006n9n
Title : Crystal structure of murine GSDMD
Authors : Liu, Z.; Wang, C.; Yang, J.; Xiao, T.S.
Deposited on : 2018-12-03
Resolution : 3.30 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

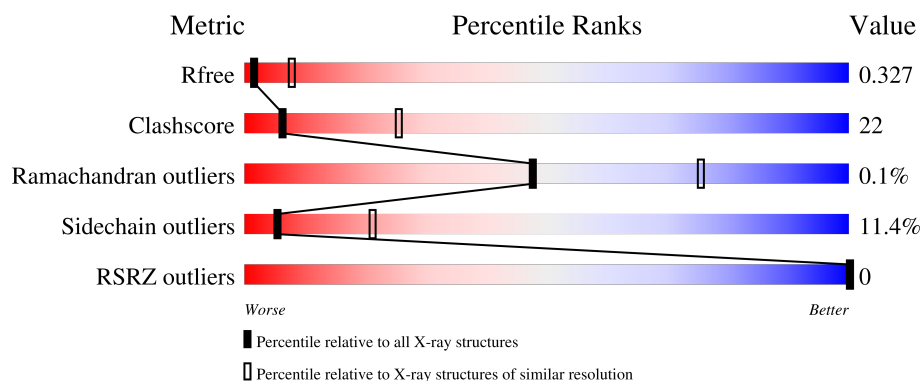
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	488	
1	B	488	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5954 atoms, of which 0 are hydrogens and 0 are deuteriums.

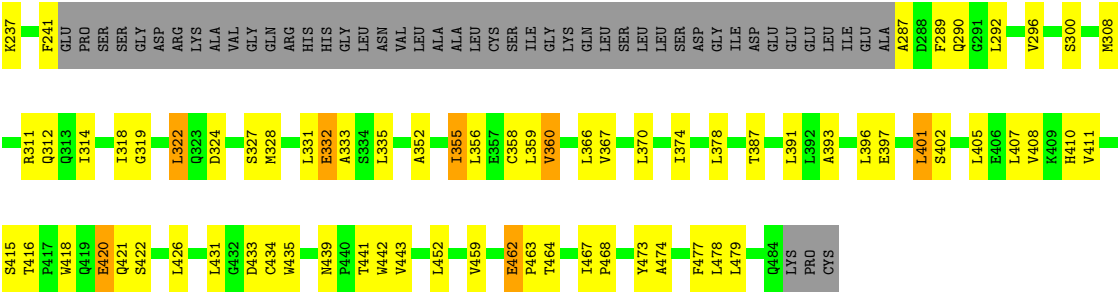
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Gasdermin-D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	0	0	0
			2945	1869	493	568	15			
1	B	388	Total	C	N	O	S	0	0	0
			3009	1906	503	585	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q9D8T2
B	0	SER	-	expression tag	UNP Q9D8T2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.42Å 86.84Å 83.54Å 90.00° 95.27° 90.00°	Depositor
Resolution (Å)	46.01 – 3.30 46.01 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.01-3.30) 99.6 (46.01-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 3.32Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, R_{free}	0.261 , 0.321 0.269 , 0.327	Depositor DCC
R_{free} test set	697 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	139.8	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 127.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5954	wwPDB-VP
Average B, all atoms (Å ²)	152.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.10% 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	0.53	0/2991	0.80	0/4053
1	B	0.46	0/3054	0.71	0/4136
All	All	0.49	0/6045	0.76	0/8189

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 [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	2945	0	2998	151	0
1	B	3009	0	3051	119	0
All	All	5954	0	6049	266	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 22.

All (266) 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:319:GLY:HA2	1:A:322:LEU:HD12	1.21	1.16
1:A:67:GLU:CB	1:A:68:PRO:HD3	1.75	1.13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ILE:O	1:A:322:LEU:HG	1.48	1.10
1:A:319:GLY:HA2	1:A:322:LEU:CD1	1.87	1.03
1:A:67:GLU:HB2	1:A:68:PRO:HD3	1.40	1.00
1:A:67:GLU:CB	1:A:68:PRO:CD	2.43	0.97
1:A:335:LEU:HD12	1:A:378:LEU:HD12	1.44	0.96
1:A:67:GLU:HB3	1:A:68:PRO:HD3	1.47	0.96
1:A:67:GLU:HB2	1:A:68:PRO:CD	1.96	0.95
1:A:335:LEU:CD1	1:A:378:LEU:HD12	2.00	0.91
1:B:12:VAL:HG13	1:B:95:VAL:HG21	1.55	0.87
1:A:407:LEU:HD11	1:A:431:LEU:HD21	1.58	0.86
1:A:144:GLU:HG3	1:A:148:LEU:HB2	1.60	0.82
1:A:335:LEU:HD12	1:A:378:LEU:CD1	2.09	0.82
1:A:39:CYS:SG	1:A:40:LEU:N	2.56	0.78
1:A:66:LEU:CD2	1:A:140:LEU:HA	2.16	0.76
1:A:123:ILE:HG22	1:A:165:LEU:HG	1.67	0.74
1:A:66:LEU:O	1:A:141:GLN:HB2	1.86	0.74
1:A:40:LEU:HD23	1:A:158:LEU:HD21	1.70	0.74
1:A:407:LEU:HD12	1:A:441:THR:HG21	1.70	0.73
1:A:124:LEU:HB2	1:A:164:VAL:HG12	1.71	0.72
1:B:43:ARG:HG3	1:B:53:PRO:HG2	1.72	0.72
1:B:159:PHE:HD1	1:B:221:GLN:HA	1.56	0.70
1:B:332:GLU:HA	1:B:335:LEU:HD12	1.74	0.70
1:B:152:ARG:NH2	1:B:241:PHE:O	2.25	0.70
1:A:237:LYS:HE3	1:A:238:GLN:HG3	1.74	0.70
1:B:332:GLU:HB3	1:B:378:LEU:HD23	1.73	0.70
1:B:367:VAL:HB	1:B:370:LEU:HB2	1.73	0.68
1:A:303:LEU:HD23	1:A:482:LEU:HD21	1.74	0.68
1:B:166:GLN:HB3	1:B:214:ILE:HD13	1.75	0.68
1:A:62:ILE:HG22	1:A:83:VAL:HG21	1.77	0.66
1:A:2:PRO:O	1:A:7:LYS:HE2	1.96	0.65
1:A:221:GLN:O	1:A:231:LEU:HB2	1.95	0.65
1:A:452:LEU:HD22	1:A:459:VAL:HG12	1.79	0.65
1:A:474:ALA:O	1:A:478:LEU:HD22	1.97	0.64
1:A:222:LEU:HD12	1:A:222:LEU:H	1.62	0.64
1:A:296:VAL:HG11	1:A:474:ALA:HA	1.80	0.64
1:A:66:LEU:HD23	1:A:140:LEU:HA	1.78	0.64
1:A:87:VAL:HG11	1:A:127:THR:HG22	1.81	0.62
1:A:66:LEU:HD22	1:A:140:LEU:HA	1.80	0.62
1:A:34:SER:HB3	1:A:57:CYS:SG	2.41	0.61
1:A:306:LEU:HB3	1:A:310:LEU:HD23	1.82	0.61
1:A:133:THR:O	1:A:137:GLU:N	2.31	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:ILE:HG12	1:B:355:ILE:HG22	1.82	0.61
1:A:97:LEU:HD22	1:A:98:SER:H	1.64	0.61
1:A:315:LEU:HD11	1:A:482:LEU:HB2	1.83	0.60
1:A:83:VAL:HG12	1:A:84:SER:H	1.66	0.60
1:A:45:PHE:HE1	1:A:239:ARG:NE	1.99	0.60
1:A:224:ILE:HG22	1:A:225:GLY:H	1.66	0.60
1:A:335:LEU:CD1	1:A:378:LEU:CD1	2.73	0.60
1:A:135:GLN:HA	1:A:228:TRP:CZ2	2.37	0.59
1:A:171:VAL:HG22	1:A:209:ILE:HB	1.82	0.59
1:A:148:LEU:O	1:A:152:ARG:HG2	2.01	0.59
1:A:386:GLU:O	1:A:390:GLN:HG2	2.03	0.59
1:A:405:LEU:HD12	1:A:477:PHE:HA	1.83	0.59
1:B:86:VAL:HG13	1:B:125:ARG:O	2.02	0.59
1:A:90:ASN:HB3	1:B:93:GLY:H	1.66	0.59
1:B:40:LEU:HD11	1:B:62:ILE:HD12	1.83	0.59
1:A:322:LEU:HD13	1:A:393:ALA:HA	1.85	0.59
1:A:332:GLU:HG2	1:A:378:LEU:HB3	1.83	0.59
1:B:314:ILE:HA	1:B:355:ILE:HG22	1.85	0.58
1:B:61:SER:OG	1:B:62:ILE:N	2.36	0.58
1:A:88:ASP:OD1	1:B:94:ARG:HG3	2.04	0.58
1:A:70:ALA:HB2	1:A:138:ARG:HH12	1.69	0.57
1:B:411:VAL:O	1:B:415:SER:N	2.37	0.57
1:A:381:LEU:HA	1:A:384:LEU:HD13	1.87	0.57
1:A:41:LEU:HD23	1:A:57:CYS:HA	1.87	0.56
1:A:392:LEU:HD21	1:A:479:LEU:HD12	1.87	0.56
1:B:86:VAL:HG22	1:B:126:VAL:HG13	1.85	0.56
1:B:435:TRP:NE1	1:B:442:TRP:HE3	2.04	0.56
1:A:467:ILE:HB	1:A:468:PRO:HD3	1.86	0.55
1:A:43:ARG:HG3	1:A:53:PRO:O	2.05	0.55
1:A:116:SER:OG	1:A:117:ALA:N	2.25	0.55
1:B:41:LEU:HD12	1:B:55:TYR:HB3	1.88	0.55
1:B:236:GLU:H	1:B:236:GLU:CD	2.15	0.55
1:B:435:TRP:CH2	1:B:441:THR:HB	2.41	0.55
1:B:50:PHE:O	1:B:51:TRP:HD1	1.88	0.55
1:A:450:LEU:HD22	1:A:461:TRP:HA	1.88	0.54
1:A:311:ARG:HH21	1:A:482:LEU:HD23	1.73	0.54
1:B:63:LYS:HD3	1:B:82:LYS:HB3	1.89	0.54
1:A:315:LEU:HD21	1:A:482:LEU:O	2.08	0.54
1:B:44:LYS:HA	1:B:156:ASP:CG	2.33	0.54
1:A:377:LEU:HD13	1:A:478:LEU:HB2	1.90	0.54
1:B:40:LEU:HD12	1:B:61:SER:O	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ILE:HD13	1:A:25:PRO:HB3	1.89	0.54
1:A:37:PRO:O	1:A:38:TYR:HB2	2.08	0.54
1:B:402:SER:O	1:B:405:LEU:HB3	2.09	0.53
1:A:24:ILE:HD12	1:A:219:VAL:HG13	1.91	0.53
1:A:158:LEU:O	1:A:222:LEU:HD12	2.08	0.53
1:A:359:LEU:HD12	1:A:370:LEU:HG	1.91	0.53
1:B:319:GLY:HA3	1:B:396:LEU:HD22	1.89	0.53
1:A:160:VAL:HG23	1:A:222:LEU:HG	1.91	0.53
1:A:435:TRP:CH2	1:A:458:GLN:HB3	2.43	0.53
1:B:408:VAL:HA	1:B:411:VAL:HG12	1.89	0.53
1:A:135:GLN:NE2	1:A:229:ASP:HB3	2.23	0.52
1:B:467:ILE:HB	1:B:468:PRO:HD3	1.90	0.52
1:A:384:LEU:HG	1:A:388:GLN:HE21	1.75	0.52
1:A:466:LEU:O	1:A:470:SER:HB2	2.09	0.52
1:A:5:PHE:CE1	1:A:29:LEU:HD12	2.45	0.52
1:B:43:ARG:NH2	1:B:52:LYS:HG3	2.23	0.52
1:A:2:PRO:HA	1:A:6:GLU:HB2	1.91	0.52
1:B:387:THR:O	1:B:391:LEU:HG	2.09	0.52
1:B:19:SER:H	1:B:218:ARG:HH22	1.56	0.51
1:B:435:TRP:HE1	1:B:442:TRP:HE3	1.58	0.51
1:A:391:LEU:HD23	1:A:444:LEU:HD21	1.92	0.51
1:A:392:LEU:HD23	1:A:392:LEU:O	2.10	0.51
1:A:404:GLN:HB3	1:A:476:LEU:HD13	1.92	0.51
1:B:45:PHE:HD2	1:B:47:SER:HG	1.58	0.51
1:A:43:ARG:HD3	1:A:53:PRO:HD2	1.92	0.51
1:B:229:ASP:OD1	1:B:229:ASP:N	2.44	0.51
1:B:356:LEU:O	1:B:360:VAL:HG23	2.10	0.51
1:A:126:VAL:HG13	1:A:131:TRP:HE1	1.74	0.51
1:B:164:VAL:HG12	1:B:217:PHE:HB3	1.93	0.51
1:B:5:PHE:CD1	1:B:5:PHE:C	2.89	0.51
1:A:142:GLN:O	1:A:144:GLU:N	2.40	0.51
1:A:355:ILE:O	1:A:359:LEU:HD22	2.11	0.50
1:B:174:THR:HA	1:B:206:MET:HA	1.93	0.50
1:B:148:LEU:HD11	1:B:224:ILE:HD12	1.93	0.50
1:B:415:SER:OG	1:B:418:TRP:NE1	2.31	0.50
1:B:435:TRP:CD1	1:B:442:TRP:HE3	2.30	0.50
1:A:475:SER:O	1:A:479:LEU:HG	2.12	0.49
1:B:442:TRP:CZ2	1:B:452:LEU:HB2	2.47	0.49
1:A:28:SER:OG	1:A:30:ARG:HG3	2.12	0.49
1:A:134:MET:HA	1:A:137:GLU:HB3	1.95	0.49
1:A:164:VAL:HG21	1:A:214:ILE:HD13	1.92	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:LYS:HD3	1:B:332:GLU:HG3	1.95	0.49
1:B:150:GLN:O	1:B:153:SER:HB3	2.12	0.49
1:B:462:GLU:HB3	1:B:464:THR:HG22	1.94	0.49
1:A:40:LEU:HD23	1:A:158:LEU:CD2	2.41	0.49
1:A:478:LEU:HA	1:A:481:SER:HB3	1.95	0.49
1:B:308:MET:HG3	1:B:311:ARG:NH2	2.27	0.49
1:A:290:GLN:OE1	1:A:290:GLN:N	2.45	0.49
1:B:311:ARG:HH12	1:B:312:GLN:NE2	2.11	0.49
1:B:405:LEU:HD22	1:B:477:PHE:HA	1.95	0.49
1:A:90:ASN:HB3	1:B:93:GLY:N	2.27	0.49
1:B:145:ASN:HB2	1:B:149:GLN:HB2	1.94	0.49
1:B:147:ILE:HD12	1:B:148:LEU:H	1.77	0.49
1:B:327:SER:HB3	1:B:352:ALA:HB2	1.94	0.49
1:A:205:LYS:HE2	1:A:207:VAL:HG13	1.95	0.49
1:A:3:SER:OG	1:A:4:ALA:N	2.45	0.48
1:A:49:ARG:HG3	1:A:50:PHE:CE1	2.47	0.48
1:A:87:VAL:HG22	1:A:88:ASP:H	1.79	0.48
1:B:407:LEU:O	1:B:410:HIS:HB3	2.13	0.48
1:A:325:GLN:NE2	1:A:389:GLN:OE1	2.46	0.48
1:A:64:ASP:OD1	1:A:64:ASP:N	2.35	0.48
1:B:45:PHE:O	1:B:46:SER:OG	2.25	0.48
1:A:116:SER:HG	1:A:117:ALA:H	1.55	0.48
1:B:46:SER:HB3	1:B:53:PRO:HG3	1.95	0.47
1:B:314:ILE:HD11	1:B:358:CYS:HB2	1.95	0.47
1:A:29:LEU:O	1:A:29:LEU:HD23	2.15	0.47
1:A:148:LEU:HD13	1:A:148:LEU:HA	1.67	0.47
1:B:452:LEU:HD22	1:B:459:VAL:HG22	1.95	0.47
1:B:146:LYS:HB2	1:B:146:LYS:HE2	1.47	0.47
1:A:36:ARG:O	1:A:39:CYS:HB3	2.15	0.47
1:A:40:LEU:HD13	1:A:61:SER:O	2.14	0.47
1:A:321:ILE:HG23	1:A:351:PRO:HB2	1.97	0.47
1:B:140:LEU:H	1:B:140:LEU:HG	1.46	0.47
1:A:83:VAL:HG12	1:A:84:SER:N	2.29	0.47
1:A:91:ILE:O	1:B:91:ILE:O	2.32	0.47
1:B:84:SER:O	1:B:85:ASP:HB2	2.15	0.47
1:A:63:LYS:H	1:A:63:LYS:HG3	1.54	0.46
1:B:84:SER:OG	1:B:85:ASP:N	2.47	0.46
1:B:322:LEU:HB3	1:B:393:ALA:HB2	1.98	0.46
1:B:135:GLN:HA	1:B:228:TRP:CZ2	2.51	0.46
1:A:167:THR:HG22	1:A:213:SER:O	2.15	0.46
1:A:328:MET:HE1	1:A:389:GLN:HE22	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:LEU:HA	1:B:23:LEU:HD12	1.54	0.46
1:B:44:LYS:HA	1:B:156:ASP:OD1	2.16	0.46
1:A:444:LEU:O	1:A:448:CYS:HB2	2.16	0.46
1:A:92:GLN:O	1:A:93:GLY:C	2.59	0.46
1:A:222:LEU:HD12	1:A:222:LEU:N	2.29	0.46
1:A:325:GLN:O	1:A:328:MET:N	2.48	0.46
1:A:128:GLN:O	1:A:128:GLN:HG2	2.15	0.46
1:A:435:TRP:HZ3	1:A:454:VAL:HA	1.80	0.46
1:B:290:GLN:OE1	1:B:290:GLN:N	2.48	0.45
1:A:38:TYR:HB3	1:A:83:VAL:HG21	1.98	0.45
1:A:451:ARG:HD2	1:A:452:LEU:H	1.81	0.45
1:A:465:SER:HA	1:A:468:PRO:HD2	1.98	0.45
1:A:67:GLU:HB3	1:A:68:PRO:CD	2.29	0.45
1:A:220:ALA:HB1	1:A:230:ILE:HG22	1.97	0.45
1:B:97:LEU:HD11	1:B:119:MET:HE2	1.98	0.45
1:B:296:VAL:HG21	1:B:474:ALA:HA	1.98	0.45
1:A:224:ILE:HG22	1:A:225:GLY:N	2.31	0.45
1:A:296:VAL:HG12	1:A:477:PHE:HD2	1.81	0.45
1:A:304:GLU:OE2	1:A:484:GLN:NE2	2.49	0.45
1:B:105:ILE:HD13	1:B:173:ILE:HD11	1.99	0.45
1:B:405:LEU:HD11	1:B:477:PHE:HD1	1.80	0.45
1:A:322:LEU:CD1	1:A:393:ALA:HA	2.47	0.45
1:B:142:GLN:O	1:B:144:GLU:N	2.41	0.45
1:B:296:VAL:HG11	1:B:473:TYR:CE2	2.51	0.45
1:B:401:LEU:HD13	1:B:479:LEU:HD12	1.99	0.45
1:A:348:LEU:O	1:A:353:GLY:HA3	2.17	0.45
1:A:91:ILE:C	1:A:93:GLY:H	2.25	0.45
1:B:231:LEU:HD23	1:B:231:LEU:HA	1.71	0.45
1:B:29:LEU:HG	1:B:30:ARG:NH1	2.33	0.44
1:A:311:ARG:HE	1:A:482:LEU:HA	1.83	0.44
1:B:10:LYS:O	1:B:13:ILE:HG13	2.16	0.44
1:A:303:LEU:HD23	1:A:482:LEU:HD11	1.99	0.44
1:B:160:VAL:HG12	1:B:222:LEU:HD22	1.99	0.44
1:B:224:ILE:HD11	1:B:241:PHE:CE1	2.53	0.44
1:A:311:ARG:NH2	1:A:482:LEU:HD23	2.32	0.44
1:B:420:GLU:OE1	1:B:422:SER:HB3	2.18	0.44
1:A:476:LEU:O	1:A:480:SER:HB3	2.18	0.44
1:B:156:ASP:O	1:B:241:PHE:HE2	2.01	0.44
1:B:415:SER:HG	1:B:418:TRP:HE1	1.61	0.44
1:B:120:ASN:HB2	1:B:169:GLU:HG2	1.99	0.43
1:B:308:MET:O	1:B:312:GLN:HG2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:THR:O	1:A:212:GLY:N	2.47	0.43
1:A:385:SER:O	1:A:389:GLN:HG2	2.18	0.43
1:B:29:LEU:CD1	1:B:30:ARG:HD3	2.48	0.43
1:B:41:LEU:HA	1:B:58:VAL:HG23	2.00	0.43
1:A:43:ARG:NH1	1:A:52:LYS:HD2	2.33	0.43
1:A:49:ARG:HG2	1:A:295:GLU:OE2	2.18	0.43
1:B:314:ILE:O	1:B:318:ILE:HG12	2.18	0.43
1:B:328:MET:HB3	1:B:378:LEU:HD11	2.00	0.43
1:A:405:LEU:HD11	1:A:477:PHE:CD1	2.53	0.43
1:A:145:ASN:O	1:A:149:GLN:HB3	2.19	0.43
1:B:431:LEU:HB3	1:B:435:TRP:CE3	2.53	0.43
1:A:307:GLU:O	1:A:311:ARG:HG3	2.19	0.43
1:B:431:LEU:O	1:B:435:TRP:HE3	2.02	0.43
1:A:331:LEU:HA	1:A:331:LEU:HD12	1.73	0.43
1:B:141:GLN:O	1:B:144:GLU:HB3	2.19	0.43
1:A:92:GLN:HB3	1:A:121:VAL:HG23	2.00	0.42
1:A:95:VAL:HG22	1:A:119:MET:O	2.18	0.42
1:A:411:VAL:HG22	1:A:426:LEU:HD21	2.02	0.42
1:B:58:VAL:HG12	1:B:60:LEU:HD23	2.01	0.42
1:A:378:LEU:HD23	1:A:378:LEU:HA	1.93	0.42
1:B:50:PHE:CZ	1:B:287:ALA:HA	2.55	0.42
1:B:81:PHE:HB2	1:B:83:VAL:O	2.20	0.42
1:B:145:ASN:HA	1:B:149:GLN:HB2	2.01	0.42
1:B:435:TRP:HH2	1:B:441:THR:HB	1.84	0.42
1:A:22:ASP:O	1:A:218:ARG:HG3	2.19	0.42
1:A:159:PHE:HD1	1:A:221:GLN:HB2	1.85	0.42
1:B:439:ASN:O	1:B:443:VAL:HG23	2.20	0.42
1:B:170:GLU:HG3	1:B:210:PRO:HA	2.01	0.42
1:B:360:VAL:HG22	1:B:366:LEU:HD21	2.00	0.42
1:A:87:VAL:HG22	1:A:88:ASP:N	2.34	0.42
1:B:289:PHE:CD2	1:B:292:LEU:HD23	2.55	0.42
1:B:318:ILE:HD13	1:B:318:ILE:HA	1.77	0.42
1:B:401:LEU:HG	1:B:402:SER:N	2.35	0.42
1:B:159:PHE:HD1	1:B:221:GLN:CA	2.30	0.42
1:A:169:GLU:O	1:A:171:VAL:HG13	2.20	0.41
1:B:322:LEU:HA	1:B:322:LEU:HD12	1.84	0.41
1:B:43:ARG:CG	1:B:53:PRO:HG2	2.47	0.41
1:B:324:ASP:OD2	1:B:327:SER:OG	2.33	0.41
1:B:421:GLN:HG2	1:B:463:PRO:HD3	2.01	0.41
1:A:435:TRP:CZ3	1:A:454:VAL:HA	2.55	0.41
1:B:148:LEU:CD1	1:B:224:ILE:HD12	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:GLU:HB2	1:A:68:PRO:HD2	1.92	0.41
1:A:58:VAL:O	1:A:58:VAL:HG12	2.20	0.41
1:B:151:LEU:HD23	1:B:151:LEU:HA	1.83	0.41
1:B:331:LEU:HD12	1:B:331:LEU:HA	1.71	0.41
1:B:355:ILE:H	1:B:355:ILE:HG12	1.68	0.41
1:A:116:SER:HG	1:A:117:ALA:N	2.16	0.41
1:A:450:LEU:HD21	1:A:465:SER:HB2	2.03	0.41
1:B:300:SER:HB3	1:B:478:LEU:CD2	2.51	0.41
1:B:426:LEU:HD12	1:B:431:LEU:HD11	2.03	0.41
1:A:435:TRP:CZ3	1:A:458:GLN:HG2	2.55	0.40
1:A:126:VAL:HG12	1:A:162:THR:O	2.21	0.40
1:B:135:GLN:HA	1:B:228:TRP:HZ2	1.86	0.40
1:B:359:LEU:HD13	1:B:374:ILE:HD13	2.02	0.40
1:B:92:GLN:HB2	1:B:121:VAL:HG22	2.03	0.40
1:A:92:GLN:HB3	1:A:121:VAL:CG2	2.51	0.40
1:A:49:ARG:HG3	1:A:50:PHE:CD1	2.57	0.40
1:B:43:ARG:HH22	1:B:52:LYS:HE3	1.85	0.40
1:B:332:GLU:HG2	1:B:333:ALA:N	2.36	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	368/488 (75%)	337 (92%)	30 (8%)	1 (0%)	36	65
1	B	378/488 (78%)	345 (91%)	33 (9%)	0	100	100
All	All	746/976 (76%)	682 (91%)	63 (8%)	1 (0%)	48	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	GLU

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	339/424 (80%)	304 (90%)	35 (10%)	7	25
1	B	345/424 (81%)	302 (88%)	43 (12%)	4	19
All	All	684/848 (81%)	606 (89%)	78 (11%)	5	21

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	26	VAL
1	A	34	SER
1	A	40	LEU
1	A	49	ARG
1	A	56	SER
1	A	61	SER
1	A	86	VAL
1	A	90	ASN
1	A	91	ILE
1	A	92	GLN
1	A	97	LEU
1	A	120	ASN
1	A	126	VAL
1	A	127	THR
1	A	136	HIS
1	A	140	LEU
1	A	158	LEU
1	A	164	VAL
1	A	171	VAL
1	A	206	MET
1	A	219	VAL
1	A	222	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	315	LEU
1	A	359	LEU
1	A	363	SER
1	A	394	LYS
1	A	430	LEU
1	A	434	CYS
1	A	438	LYS
1	A	448	CYS
1	A	462	GLU
1	A	478	LEU
1	A	480	SER
1	A	481	SER
1	B	5	PHE
1	B	9	VAL
1	B	41	LEU
1	B	60	LEU
1	B	63	LYS
1	B	83	VAL
1	B	90	ASN
1	B	91	ILE
1	B	92	GLN
1	B	94	ARG
1	B	95	VAL
1	B	97	LEU
1	B	111	VAL
1	B	121	VAL
1	B	127	THR
1	B	136	HIS
1	B	139	HIS
1	B	140	LEU
1	B	141	GLN
1	B	144	GLU
1	B	146	LYS
1	B	147	ILE
1	B	148	LEU
1	B	164	VAL
1	B	171	VAL
1	B	174	THR
1	B	206	MET
1	B	215	LEU
1	B	224	ILE
1	B	232	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	234	SER
1	B	237	LYS
1	B	322	LEU
1	B	332	GLU
1	B	355	ILE
1	B	360	VAL
1	B	397	GLU
1	B	401	LEU
1	B	416	THR
1	B	420	GLU
1	B	433	ASP
1	B	434	CYS
1	B	462	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	92	GLN
1	A	141	GLN
1	A	388	GLN
1	A	484	GLN
1	B	90	ASN
1	B	92	GLN
1	B	149	GLN
1	B	238	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 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 [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	378/488 (77%)	-0.40	0 100 100	92, 133, 176, 195	0
1	B	388/488 (79%)	-0.31	0 100 100	95, 174, 212, 222	0
All	All	766/976 (78%)	-0.36	0 100 100	92, 150, 207, 222	0

There are no RSRZ outliers to report.

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 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.