



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:40 PM UTC

PDB ID : 4G1O / pdb_00004g1o
Title : Crystal structure of Newcastle disease virus matrix protein
Authors : Meng, G.; Rossmann, M.G.
Deposited on : 2012-07-11
Resolution : 2.20 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

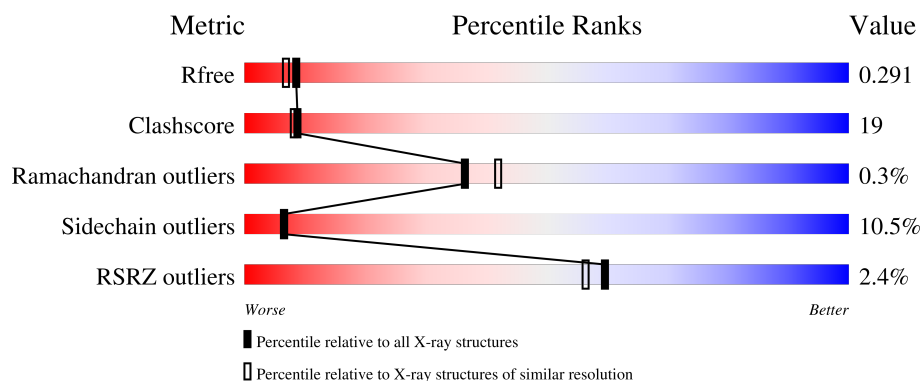
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	364	2% 60% 24% . . 10%
1	B	364	2% 63% 19% 7% . 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5089 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 Matrix protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2517	1610	437	461	9			
1	B	326	Total	C	N	O	S	0	0	0
			2501	1600	436	456	9			

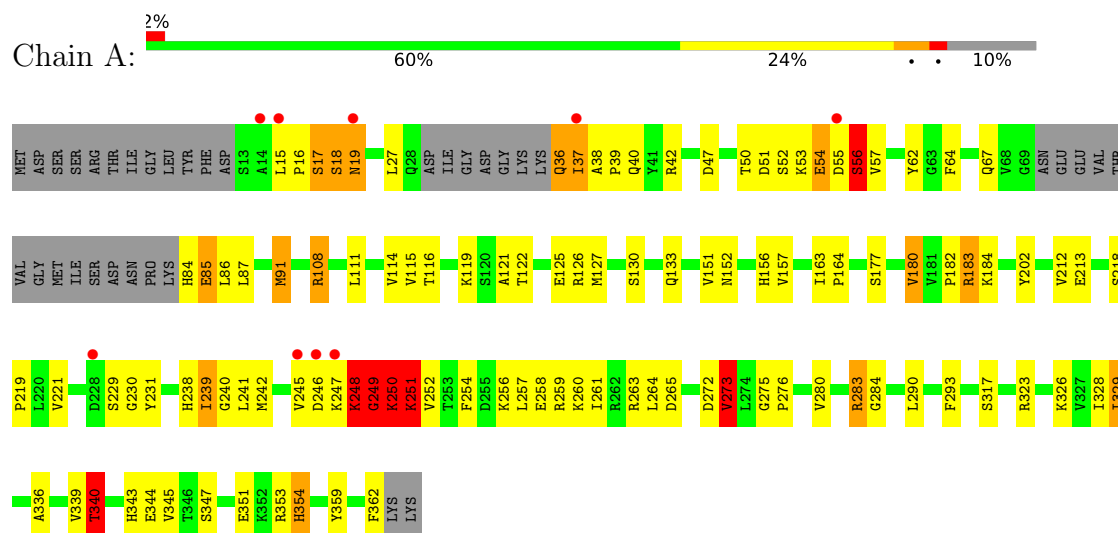
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	33	Total	O	0	0
			33	33		
2	B	38	Total	O	0	0
			38	38		

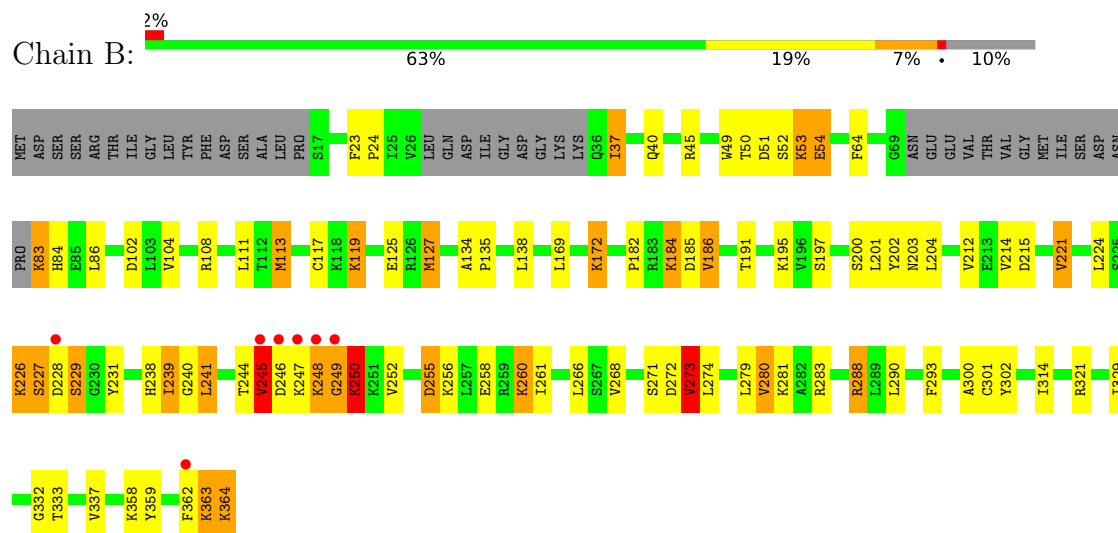
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Matrix protein



• Molecule 1: Matrix protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	163.31Å 46.99Å 117.41Å 90.00° 132.05° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 30.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (30.00-2.20) 99.4 (30.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.26 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.180 , 0.280 0.194 , 0.291	Depositor DCC
R_{free} test set	1693 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	47.2	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5089	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% 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	0.95	4/2560 (0.2%)	1.20	12/3471 (0.3%)
1	B	0.95	1/2543 (0.0%)	1.15	11/3443 (0.3%)
All	All	0.95	5/5103 (0.1%)	1.18	23/6914 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	251	LYS	CA-C	-6.68	1.47	1.53
1	A	250	LYS	N-CA	-5.99	1.38	1.46
1	A	238	HIS	CG-CD2	5.54	1.42	1.35
1	A	354	HIS	CG-CD2	5.18	1.41	1.35
1	B	49	TRP	NE1-CE2	-5.12	1.31	1.37

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	250	LYS	N-CA-C	-12.19	90.60	109.85
1	B	248	LYS	N-CA-C	-12.00	98.22	112.86
1	A	56	SER	N-CA-C	11.06	124.00	108.74
1	A	250	LYS	N-CA-C	-10.61	91.61	108.90
1	A	230	GLY	CA-C-N	-9.38	107.98	122.62
1	A	230	GLY	C-N-CA	-9.38	107.98	122.62
1	A	17	SER	CB-CA-C	-8.78	97.41	110.06
1	A	249	GLY	N-CA-C	8.69	124.81	112.81
1	B	273	VAL	CB-CA-C	-8.10	98.00	111.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	SER	N-CA-CB	-7.71	98.34	111.21
1	A	248	LYS	N-CA-C	-7.23	101.97	111.74
1	B	249	GLY	N-CA-C	-7.12	96.30	113.18
1	A	18	SER	N-CA-C	-7.09	103.61	112.90
1	B	186	VAL	CB-CA-C	6.74	120.36	112.68
1	B	229	SER	N-CA-C	6.25	118.09	111.28
1	A	230	GLY	O-C-N	6.23	131.15	122.55
1	B	302	TYR	CA-C-N	-5.99	113.62	119.90
1	B	302	TYR	C-N-CA	-5.99	113.62	119.90
1	A	340	THR	CB-CA-C	5.50	119.28	110.16
1	B	261	ILE	N-CA-C	5.29	116.01	110.62
1	B	245	VAL	N-CA-C	5.26	115.42	107.80
1	B	113	MET	CG-SD-CE	-5.22	89.41	100.90
1	A	273	VAL	CB-CA-C	-5.16	102.83	111.29

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	249	GLY	Mainchain
1	A	250	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2517	0	2630	103	0
1	B	2501	0	2622	91	0
2	A	33	0	0	0	0
2	B	38	0	0	0	0
All	All	5089	0	5252	192	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 19.

All (192) 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:16:PRO:HG2	1:A:19:ASN:OD1	1.47	1.13
1:B:288:ARG:HG2	1:B:288:ARG:HH11	1.02	1.11
1:B:182:PRO:HB3	1:B:184:LYS:HE2	1.34	1.04
1:A:54:GLU:OE1	1:A:180:VAL:HG12	1.56	1.04
1:A:15:LEU:HB3	1:A:16:PRO:HD2	1.40	1.00
1:A:245:VAL:HG12	1:A:251:LYS:H	1.25	1.00
1:A:183:ARG:HH11	1:A:183:ARG:HG3	1.32	0.91
1:A:259:ARG:HH11	1:A:263:ARG:HH12	1.02	0.91
1:B:50:THR:HG22	1:B:52:SER:H	1.37	0.90
1:B:247:LYS:O	1:B:248:LYS:HG2	1.71	0.90
1:B:288:ARG:HG2	1:B:288:ARG:NH1	1.80	0.89
1:A:38:ALA:O	1:A:39:PRO:C	2.16	0.88
1:A:259:ARG:HH11	1:A:263:ARG:NH1	1.72	0.87
1:A:16:PRO:O	1:A:17:SER:HB3	1.74	0.85
1:B:246:ASP:O	1:B:249:GLY:O	1.97	0.81
1:B:245:VAL:HG12	1:B:245:VAL:O	1.81	0.80
1:B:53:LYS:HD2	1:B:54:GLU:N	1.95	0.80
1:B:245:VAL:O	1:B:245:VAL:CG1	2.30	0.80
1:A:259:ARG:NH1	1:A:263:ARG:HH12	1.78	0.79
1:B:248:LYS:O	1:B:248:LYS:CG	2.30	0.79
1:A:16:PRO:O	1:A:17:SER:CB	2.30	0.78
1:A:16:PRO:HG2	1:A:19:ASN:CG	2.08	0.78
1:A:50:THR:HG22	1:A:52:SER:H	1.48	0.78
1:B:111:LEU:HD11	1:B:362:PHE:CE2	2.19	0.77
1:B:248:LYS:O	1:B:248:LYS:HG3	1.84	0.77
1:B:184:LYS:HD3	1:B:184:LYS:H	1.50	0.75
1:A:64:PHE:HB3	1:A:86:LEU:HD11	1.69	0.75
1:B:119:LYS:HE3	1:B:125:GLU:OE2	1.91	0.71
1:A:37:ILE:O	1:A:37:ILE:HG23	1.90	0.70
1:A:27:LEU:HB2	1:A:218:SER:HA	1.71	0.70
1:A:55:ASP:CG	1:A:183:ARG:H	1.98	0.70
1:B:245:VAL:HG22	1:B:249:GLY:O	1.92	0.70
1:A:55:ASP:OD2	1:A:183:ARG:HB3	1.93	0.69
1:A:183:ARG:HG3	1:A:183:ARG:NH1	2.00	0.69
1:B:247:LYS:O	1:B:248:LYS:CG	2.40	0.69
1:A:336:ALA:O	1:A:340:THR:HG23	1.93	0.68
1:A:241:LEU:O	1:A:290:LEU:CD1	2.43	0.67
1:A:258:GLU:HG3	1:A:345:VAL:HG13	1.75	0.66
1:B:227:SER:O	1:B:228:ASP:C	2.34	0.66
1:A:242:MET:HG2	1:A:290:LEU:HD11	1.78	0.65
1:A:241:LEU:O	1:A:290:LEU:HD12	1.97	0.65
1:A:252:VAL:HG13	1:A:256:LYS:HB2	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ILE:O	1:A:37:ILE:CG2	2.44	0.65
1:B:363:LYS:O	1:B:364:LYS:C	2.39	0.64
1:A:50:THR:HG22	1:A:51:ASP:N	2.11	0.64
1:A:39:PRO:HB3	1:A:111:LEU:HD11	1.80	0.64
1:A:259:ARG:NH1	1:A:263:ARG:NH1	2.43	0.64
1:A:15:LEU:HB3	1:A:16:PRO:CD	2.23	0.63
1:A:245:VAL:HG12	1:A:251:LYS:N	2.05	0.63
1:A:64:PHE:HB3	1:A:86:LEU:CD1	2.29	0.62
1:B:127:MET:HA	1:B:127:MET:HE2	1.79	0.62
1:A:55:ASP:C	1:A:56:SER:OG	2.39	0.62
1:A:157:VAL:HG11	1:A:163:ILE:CD1	2.30	0.62
1:B:53:LYS:HD2	1:B:54:GLU:H	1.65	0.62
1:A:119:LYS:HD3	1:A:127:MET:HE1	1.80	0.61
1:B:246:ASP:OD1	1:B:247:LYS:N	2.34	0.60
1:A:157:VAL:HG11	1:A:163:ILE:HD12	1.83	0.60
1:B:255:ASP:N	1:B:255:ASP:OD1	2.34	0.60
1:B:50:THR:HG22	1:B:51:ASP:N	2.17	0.59
1:B:288:ARG:HH11	1:B:288:ARG:CG	1.94	0.59
1:A:67:GLN:HB3	1:A:85:GLU:HG2	1.85	0.59
1:A:265:ASP:O	1:A:283:ARG:HD3	2.02	0.59
1:B:108:ARG:HG2	1:B:362:PHE:CE1	2.38	0.58
1:B:247:LYS:C	1:B:249:GLY:H	2.12	0.58
1:A:39:PRO:CB	1:A:111:LEU:HD11	2.33	0.58
1:B:247:LYS:C	1:B:249:GLY:N	2.54	0.58
1:B:333:THR:O	1:B:337:VAL:HG23	2.04	0.57
1:A:256:LYS:O	1:A:260:LYS:HG3	2.05	0.57
1:A:38:ALA:O	1:A:40:GLN:N	2.38	0.56
1:A:42:ARG:HE	1:A:177:SER:HB2	1.70	0.56
1:A:50:THR:CG2	1:A:51:ASP:N	2.68	0.56
1:B:226:LYS:HD2	1:B:227:SER:N	2.19	0.56
1:B:245:VAL:HG22	1:B:250:LYS:HA	1.86	0.56
1:B:247:LYS:O	1:B:248:LYS:CB	2.51	0.56
1:B:247:LYS:O	1:B:247:LYS:CG	2.52	0.56
1:A:239:ILE:HD11	1:A:280:VAL:HG21	1.87	0.55
1:B:247:LYS:O	1:B:247:LYS:HG2	2.06	0.55
1:B:53:LYS:HD2	1:B:53:LYS:C	2.24	0.55
1:B:226:LYS:HD2	1:B:226:LYS:C	2.31	0.55
1:B:50:THR:HG22	1:B:52:SER:N	2.17	0.54
1:B:37:ILE:O	1:B:37:ILE:HG23	2.07	0.54
1:A:16:PRO:CG	1:A:19:ASN:OD1	2.38	0.54
1:A:261:ILE:HD11	1:A:329:ILE:HD11	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:LYS:NZ	1:B:54:GLU:OE1	2.30	0.54
1:A:40:GLN:HB3	1:A:359:TYR:HB3	1.89	0.54
1:A:351:GLU:HG2	1:A:354:HIS:CE1	2.43	0.54
1:B:119:LYS:CE	1:B:125:GLU:OE2	2.55	0.54
1:B:23:PHE:CG	1:B:24:PRO:HA	2.43	0.53
1:A:18:SER:HG	1:A:359:TYR:HD2	1.56	0.53
1:B:119:LYS:HD3	1:B:127:MET:HE1	1.91	0.53
1:A:202:TYR:CE2	1:A:257:LEU:HD11	2.45	0.52
1:A:15:LEU:HB3	1:A:19:ASN:HD21	1.73	0.52
1:B:256:LYS:O	1:B:260:LYS:HG3	2.09	0.52
1:B:64:PHE:CD1	1:B:86:LEU:HD11	2.45	0.52
1:B:184:LYS:H	1:B:184:LYS:CD	2.20	0.52
1:A:91:MET:O	1:A:91:MET:HG3	2.10	0.52
1:A:254:PHE:CE1	1:A:258:GLU:HB2	2.46	0.51
1:B:108:ARG:CG	1:B:362:PHE:CE1	2.93	0.51
1:A:152:ASN:O	1:A:156:HIS:HD2	1.94	0.51
1:A:15:LEU:HB3	1:A:19:ASN:ND2	2.26	0.51
1:A:245:VAL:CG1	1:A:251:LYS:H	2.12	0.51
1:A:53:LYS:O	1:A:184:LYS:NZ	2.44	0.51
1:B:119:LYS:HE3	1:B:125:GLU:CD	2.35	0.51
1:A:54:GLU:HA	1:A:182:PRO:HG3	1.94	0.50
1:B:203:ASN:OD1	1:B:238:HIS:ND1	2.37	0.50
1:A:241:LEU:O	1:A:290:LEU:HD11	2.12	0.50
1:B:40:GLN:HB3	1:B:359:TYR:HB3	1.94	0.50
1:A:55:ASP:OD1	1:A:56:SER:OG	2.26	0.49
1:B:221:VAL:HG22	1:B:231:TYR:CE1	2.47	0.49
1:B:50:THR:CG2	1:B:51:ASP:N	2.75	0.49
1:B:197:SER:HB2	1:B:332:GLY:O	2.13	0.49
1:A:339:VAL:HG23	1:A:340:THR:HG22	1.94	0.49
1:A:114:VAL:HG21	1:A:133:GLN:HE21	1.78	0.49
1:B:202:TYR:HB3	1:B:329:ILE:HG23	1.95	0.49
1:A:351:GLU:HG2	1:A:354:HIS:ND1	2.27	0.48
1:A:27:LEU:HB2	1:A:219:PRO:HD3	1.96	0.48
1:A:54:GLU:HG3	1:A:55:ASP:N	2.28	0.48
1:B:226:LYS:CD	1:B:227:SER:N	2.77	0.48
1:A:272:ASP:O	1:A:273:VAL:C	2.58	0.47
1:A:242:MET:CG	1:A:290:LEU:HD11	2.42	0.47
1:B:108:ARG:NH1	1:B:362:PHE:HD1	2.12	0.47
1:B:202:TYR:HB3	1:B:329:ILE:CG2	2.44	0.47
1:B:274:LEU:HD12	1:B:301:CYS:SG	2.55	0.47
1:A:36:GLN:O	1:A:38:ALA:HB2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:THR:OG1	1:A:130:SER:HB2	2.16	0.46
1:B:246:ASP:O	1:B:249:GLY:C	2.59	0.46
1:B:247:LYS:O	1:B:248:LYS:C	2.55	0.46
1:A:353:ARG:HG3	1:A:354:HIS:CD2	2.50	0.46
1:A:343:HIS:C	1:A:343:HIS:CD2	2.94	0.46
1:A:221:VAL:HG13	1:A:231:TYR:CE1	2.51	0.46
1:B:182:PRO:CB	1:B:184:LYS:HE2	2.25	0.45
1:B:250:LYS:HB3	1:B:250:LYS:HE3	1.48	0.45
1:A:16:PRO:C	1:A:18:SER:H	2.23	0.45
1:A:328:ILE:HD13	1:A:344:GLU:HA	1.99	0.45
1:A:108:ARG:O	1:A:111:LEU:HB2	2.16	0.45
1:B:246:ASP:N	1:B:252:VAL:HG23	2.32	0.45
1:A:119:LYS:HE3	1:A:125:GLU:OE2	2.16	0.45
1:A:16:PRO:HG2	1:A:19:ASN:ND2	2.32	0.45
1:A:275:GLY:O	1:A:276:PRO:C	2.59	0.45
1:B:201:LEU:HD13	1:B:241:LEU:HG	1.99	0.44
1:B:221:VAL:HG22	1:B:231:TYR:CD1	2.52	0.44
1:A:115:VAL:HA	1:A:130:SER:O	2.17	0.44
1:A:183:ARG:HH11	1:A:183:ARG:CG	2.15	0.44
1:A:16:PRO:HD2	1:A:19:ASN:HD21	1.83	0.44
1:A:62:TYR:OH	1:A:272:ASP:OD1	2.36	0.44
1:A:246:ASP:C	1:A:249:GLY:HA3	2.43	0.44
1:A:18:SER:HB2	1:A:317:SER:O	2.18	0.44
1:B:172:LYS:HD3	1:B:172:LYS:HA	1.61	0.44
1:A:163:ILE:HA	1:A:164:PRO:HD3	1.92	0.43
1:B:268:VAL:HA	1:B:279:LEU:O	2.17	0.43
1:A:245:VAL:O	1:A:246:ASP:OD1	2.35	0.43
1:B:50:THR:HB	1:B:185:ASP:OD2	2.19	0.43
1:A:39:PRO:HB3	1:A:111:LEU:CD1	2.47	0.43
1:B:64:PHE:HB3	1:B:86:LEU:CD1	2.49	0.43
1:B:272:ASP:O	1:B:273:VAL:C	2.61	0.43
1:A:252:VAL:CG1	1:A:256:LYS:HB2	2.48	0.42
1:B:113:MET:HB2	1:B:113:MET:HE3	1.56	0.42
1:A:121:ALA:HA	1:A:126:ARG:HG3	2.00	0.42
1:B:51:ASP:N	1:B:51:ASP:OD2	2.48	0.42
1:B:280:VAL:HG22	1:B:300:ALA:HB3	2.02	0.42
1:B:83:LYS:HB3	1:B:84:HIS:H	1.72	0.42
1:B:239:ILE:HD13	1:B:239:ILE:HG21	1.57	0.42
1:A:55:ASP:OD1	1:A:56:SER:N	2.52	0.42
1:A:256:LYS:HA	1:A:256:LYS:HD3	1.87	0.42
1:A:261:ILE:CD1	1:A:329:ILE:HD11	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:LEU:HD11	1:B:362:PHE:HE2	1.78	0.42
1:B:117:CYS:O	1:B:169:LEU:HB2	2.19	0.42
1:B:200:SER:HB2	1:B:244:THR:OG1	2.19	0.42
1:B:224:LEU:HD21	1:B:314:ILE:HD13	2.02	0.42
1:B:266:LEU:HA	1:B:281:LYS:O	2.20	0.42
1:B:108:ARG:NH1	1:B:362:PHE:CD1	2.87	0.41
1:B:127:MET:HE2	1:B:127:MET:CA	2.45	0.41
1:A:122:THR:O	1:B:238:HIS:CD2	2.73	0.41
1:A:248:LYS:HD3	1:A:248:LYS:HA	1.54	0.41
1:A:351:GLU:CG	1:A:354:HIS:ND1	2.83	0.41
1:B:271:SER:HB2	1:B:279:LEU:HD11	2.02	0.41
1:A:329:ILE:HD13	1:A:345:VAL:HG21	2.01	0.41
1:B:127:MET:HE3	1:B:127:MET:HB2	1.73	0.41
1:B:102:ASP:OD1	1:B:104:VAL:HB	2.19	0.41
1:B:240:GLY:HA2	1:B:293:PHE:CD1	2.56	0.41
1:A:122:THR:O	1:B:238:HIS:HD2	2.03	0.41
1:B:214:VAL:HG22	1:B:215:ASP:O	2.20	0.41
1:A:263:ARG:O	1:A:264:LEU:C	2.64	0.41
1:A:67:GLN:HB2	1:A:87:LEU:HD11	2.03	0.41
1:A:151:VAL:HB	1:A:156:HIS:CD2	2.56	0.41
1:A:240:GLY:HA2	1:A:293:PHE:CD1	2.56	0.41
1:A:15:LEU:CB	1:A:16:PRO:HD2	2.24	0.40
1:B:113:MET:HG2	1:B:134:ALA:HA	2.03	0.40
1:B:45:ARG:HE	1:B:45:ARG:HB3	1.58	0.40
1:A:263:ARG:O	1:A:284:GLY:HA3	2.21	0.40
1:B:135:PRO:HD2	1:B:138:LEU:HD12	2.02	0.40
1:B:204:LEU:O	1:B:239:ILE:HG22	2.21	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	323/364 (89%)	308 (95%)	14 (4%)	1 (0%)	36	42
1	B	320/364 (88%)	307 (96%)	12 (4%)	1 (0%)	36	42
All	All	643/728 (88%)	615 (96%)	26 (4%)	2 (0%)	36	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	B	37	ILE

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	283/317 (89%)	255 (90%)	28 (10%)	7	8
1	B	281/317 (89%)	250 (89%)	31 (11%)	6	6
All	All	564/634 (89%)	505 (90%)	59 (10%)	6	6

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	37	ILE
1	A	47	ASP
1	A	54	GLU
1	A	56	SER
1	A	57	VAL
1	A	84	HIS
1	A	85	GLU
1	A	91	MET
1	A	108	ARG
1	A	180	VAL
1	A	183	ARG
1	A	212	VAL
1	A	213	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	229	SER
1	A	239	ILE
1	A	247	LYS
1	A	248	LYS
1	A	250	LYS
1	A	251	LYS
1	A	273	VAL
1	A	283	ARG
1	A	323	ARG
1	A	326	LYS
1	A	329	ILE
1	A	340	THR
1	A	347	SER
1	A	362	PHE
1	B	53	LYS
1	B	54	GLU
1	B	83	LYS
1	B	119	LYS
1	B	127	MET
1	B	172	LYS
1	B	184	LYS
1	B	186	VAL
1	B	191	THR
1	B	195	LYS
1	B	212	VAL
1	B	221	VAL
1	B	226	LYS
1	B	227	SER
1	B	229	SER
1	B	239	ILE
1	B	241	LEU
1	B	245	VAL
1	B	250	LYS
1	B	255	ASP
1	B	258	GLU
1	B	260	LYS
1	B	273	VAL
1	B	280	VAL
1	B	283	ARG
1	B	288	ARG
1	B	290	LEU
1	B	321	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	358	LYS
1	B	363	LYS
1	B	364	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	28	GLN
1	A	67	GLN
1	A	133	GLN
1	A	146	ASN
1	A	156	HIS
1	A	310	GLN
1	A	334	GLN
1	A	343	HIS
1	B	19	ASN
1	B	84	HIS
1	B	234	ASN
1	B	310	GLN
1	B	334	GLN
1	B	360	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 [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	329/364 (90%)	-0.12	9 (2%) 56 53	25, 59, 98, 134	0
1	B	326/364 (89%)	-0.28	7 (2%) 63 60	25, 52, 89, 116	0
All	All	655/728 (89%)	-0.20	16 (2%) 59 56	25, 56, 95, 134	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	246	ASP	6.7
1	A	246	ASP	6.6
1	B	245	VAL	5.7
1	B	362	PHE	5.0
1	B	249	GLY	4.4
1	A	15	LEU	4.3
1	A	245	VAL	4.1
1	A	55	ASP	3.7
1	A	228	ASP	3.5
1	B	247	LYS	3.1
1	B	248	LYS	3.1
1	A	19	ASN	2.7
1	A	37	ILE	2.5
1	A	247	LYS	2.4
1	B	228	ASP	2.4
1	A	14	ALA	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 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.