



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:31 PM UTC

PDB ID : 6XY6 / pdb_00006xy6
Title : Structural insight into sheep-pox virus mediated inhibition of apoptosis
Authors : Suraweera, C.D.; Hinds, M.G.; Kvensakul, M.
Deposited on : 2020-01-29
Resolution : 2.91 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

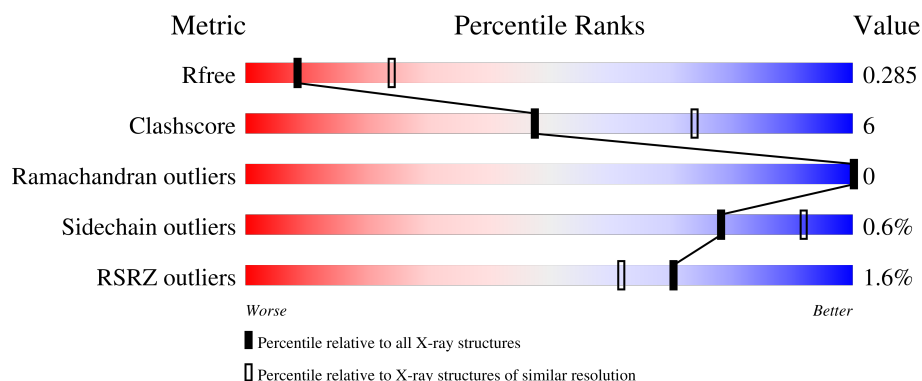
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	150	2% 77% 13% 10%
1	G	150	% 73% 17% 10%
2	B	28	4% 79% • 18%
2	D	28	82% 18%
2	F	28	4% 68% 21% 11%

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Mol	Chain	Length	Quality of chain
2	H	28	
2	J	28	
2	L	28	
2	N	28	
2	P	28	
3	C	145	
3	E	145	
3	I	145	
3	K	145	
3	M	145	
3	O	145	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20675 atoms, of which 10355 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 anti-apoptotic membrane protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	135	Total	C	H	N	O	S	0	0	0
			2240	706	1129	182	218	5			
1	G	135	Total	C	H	N	O	S	0	1	0
			2262	708	1148	182	218	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP A0A3F2YKH3
A	-3	PRO	-	expression tag	UNP A0A3F2YKH3
A	-2	LEU	-	expression tag	UNP A0A3F2YKH3
A	-1	GLY	-	expression tag	UNP A0A3F2YKH3
A	0	SER	-	expression tag	UNP A0A3F2YKH3
G	-4	GLY	-	expression tag	UNP A0A3F2YKH3
G	-3	PRO	-	expression tag	UNP A0A3F2YKH3
G	-2	LEU	-	expression tag	UNP A0A3F2YKH3
G	-1	GLY	-	expression tag	UNP A0A3F2YKH3
G	0	SER	-	expression tag	UNP A0A3F2YKH3

- Molecule 2 is a protein called Apoptosis regulator BAX.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	23	Total	C	H	N	O	S	0	0	0
			344	105	167	30	40	2			
2	D	23	Total	C	H	N	O	S	0	0	0
			349	105	172	31	39	2			
2	F	25	Total	C	H	N	O	S	0	0	0
			368	116	174	33	43	2			
2	H	24	Total	C	H	N	O	S	0	0	0
			376	112	190	32	40	2			
2	J	25	Total	C	H	N	O	S	0	0	0
			388	116	194	33	43	2			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	L	25	Total	C	H	N	O	S	0	0	0
			388	116	194	33	43	2			
2	N	22	Total	C	H	N	O	S	0	0	0
			337	100	169	29	37	2			
2	P	21	Total	C	H	N	O	S	0	0	0
			320	95	160	28	36	1			

- Molecule 3 is a protein called anti-apoptotic membrane protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	138	Total	C	H	N	O	S	0	0	0
			2301	722	1164	188	222	5			
3	E	133	Total	C	H	N	O	S	0	0	0
			2210	694	1117	178	216	5			
3	I	133	Total	C	H	N	O	S	0	0	0
			2174	694	1081	178	216	5			
3	K	134	Total	C	H	N	O	S	0	0	0
			2232	700	1130	180	217	5			
3	M	133	Total	C	H	N	O	S	0	1	0
			2218	696	1122	178	216	6			
3	O	132	Total	C	H	N	O	S	0	0	0
			2129	690	1044	176	214	5			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total O 4 4	0	0
4	B	2	Total O 2 2	0	0
4	C	5	Total O 5 5	0	0
4	E	6	Total O 6 6	0	0
4	G	3	Total O 3 3	0	0
4	H	1	Total O 1 1	0	0
4	I	4	Total O 4 4	0	0
4	K	1	Total O 1 1	0	0

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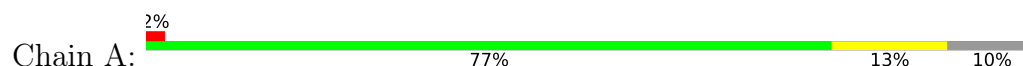
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	1	Total	O	0	0
			1	1		
4	M	6	Total	O	0	0
			6	6		
4	O	6	Total	O	0	0
			6	6		

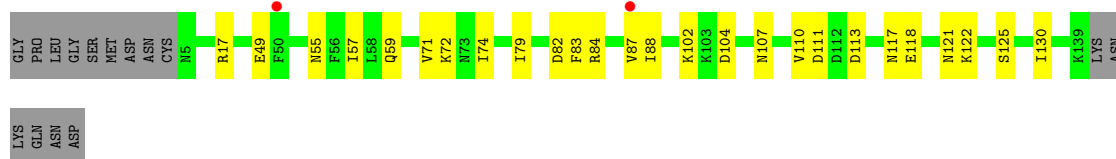
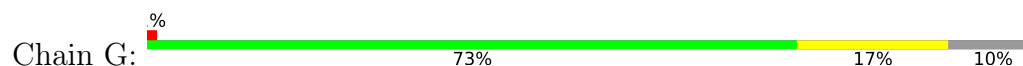
3 Residue-property plots [i](#)

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.

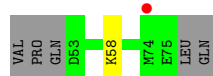
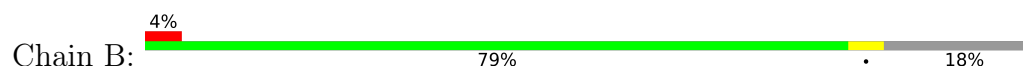
- Molecule 1: anti-apoptotic membrane protein



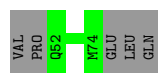
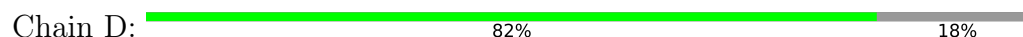
- Molecule 1: anti-apoptotic membrane protein



- Molecule 2: Apoptosis regulator BAX



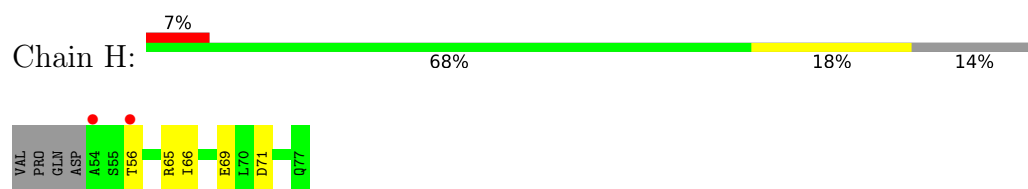
- Molecule 2: Apoptosis regulator BAX



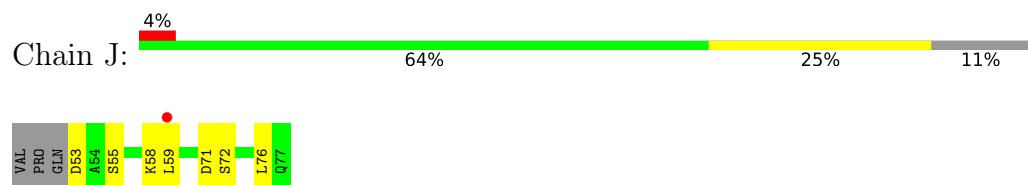
- Molecule 2: Apoptosis regulator BAX



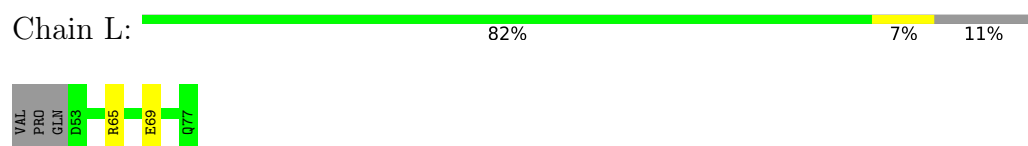
- Molecule 2: Apoptosis regulator BAX



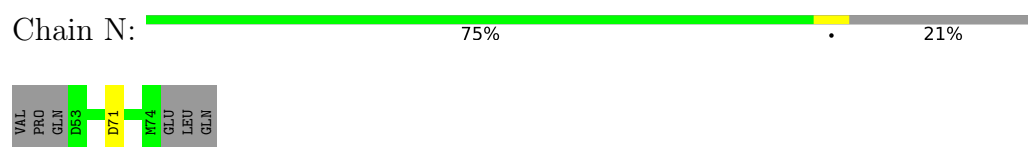
- Molecule 2: Apoptosis regulator BAX



- Molecule 2: Apoptosis regulator BAX



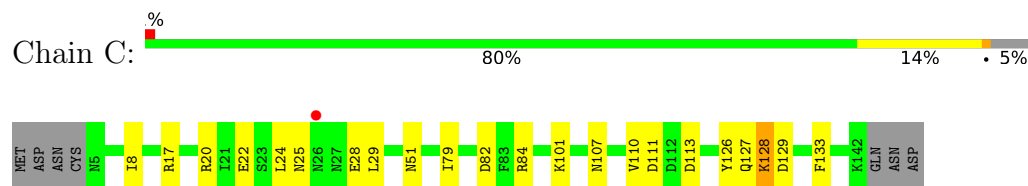
- Molecule 2: Apoptosis regulator BAX



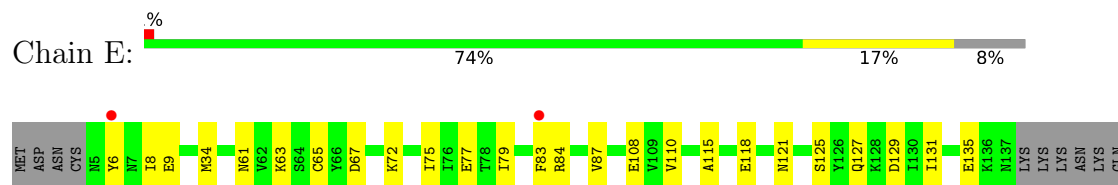
- Molecule 2: Apoptosis regulator BAX



- Molecule 3: anti-apoptotic membrane protein



- Molecule 3: anti-apoptotic membrane protein



ASN
ASP

- Molecule 3: anti-apoptotic membrane protein

Chain I:  2% 77% 14% 8%

MET	ASP	ASN	CYS	N5	I8	R17	R20	C38	F56	D67	D70	I74	F83	R84	V87	K102	N106	V110	D113	K122	S125	Y126	Q127	K128	F133	K136	N137	LYS	LYS	LYS	ASN	LYS	GLN	ASN	ASP
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- Molecule 3: anti-apoptotic membrane protein

Chain K:  0% 84% 8% 8%

MET	ASP	ASN	CYS	N5	I8	I33	T48	L58	Y66	I75	I79	N107	N117	N121	S125	Y126	Q127	K138	LYS	LYS	ASN	LYS	GLN	ASN	ASP
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- Molecule 3: anti-apoptotic membrane protein

Chain M:  0% 79% 12% 8%

MET	ASP	ASN	CYS	N5	E9	N26	L29	I33	M34	Y46	L58	V71	I79	F83	R84	K102	D112	M121	F133	V134	E135	K136	N137	LYS	LYS	LYS	ASN	LYS	GLN	ASN	ASP
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- Molecule 3: anti-apoptotic membrane protein

Chain O:  0% 77% 14% 9%

MET	ASP	ASN	CYS	ASN	Y6	W7	I8	R17	R20	E30	F56	I57	L58	K72	N80	S81	D82	F83	R84	F85	S86	K102	D112	D113	L114	A115	K122	S125	Y126	Q127	K136	N137	LYS	LYS	LYS	ASN	LYS	GLN	ASN	ASP
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.28Å 78.56Å 107.77Å 90.00° 110.97° 90.00°	Depositor
Resolution (Å)	46.82 – 2.91 46.82 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.82-2.91) 99.3 (46.82-2.91)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.239 , 0.288 0.249 , 0.285	Depositor DCC
R_{free} test set	1788 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å ²)	67.9	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20675	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.11% 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	0.16	0/1121	0.37	0/1508
1	G	0.16	0/1127	0.35	0/1516
2	B	0.15	0/176	0.30	0/232
2	D	0.14	0/176	0.33	0/232
2	F	0.18	0/193	0.41	0/255
2	H	0.16	0/185	0.42	0/244
2	J	0.16	0/193	0.41	0/255
2	L	0.14	0/193	0.37	0/255
2	N	0.15	0/167	0.32	0/220
2	P	0.15	0/159	0.40	0/210
3	C	0.17	0/1147	0.38	0/1541
3	E	0.18	0/1103	0.39	0/1486
3	I	0.15	0/1103	0.34	0/1486
3	K	0.18	0/1112	0.35	0/1497
3	M	0.19	0/1109	0.42	0/1494
3	O	0.17	0/1095	0.38	0/1475
All	All	0.17	0/10359	0.37	0/13906

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	1111	1129	1143	15	0
1	G	1114	1148	1148	18	0
2	B	177	167	175	1	0
2	D	177	172	177	0	0
2	F	194	174	194	6	0
2	H	186	190	190	4	0
2	J	194	194	194	6	0
2	L	194	194	194	1	0
2	N	168	169	169	1	0
2	P	160	160	160	4	0
3	C	1137	1164	1175	14	0
3	E	1093	1117	1117	15	0
3	I	1093	1081	1117	17	0
3	K	1102	1130	1130	7	0
3	M	1096	1122	1122	14	0
3	O	1085	1044	1111	16	0
4	A	4	0	0	0	0
4	B	2	0	0	0	0
4	C	5	0	0	0	0
4	E	6	0	0	0	0
4	G	3	0	0	0	0
4	H	1	0	0	0	0
4	I	4	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	6	0	0	0	0
4	O	6	0	0	0	0
All	All	10320	10355	10516	117	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 6.

All (117) 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)
2:L:65:ARG:NH1	2:L:69:GLU:OE2	1.97	0.97
2:F:65:ARG:NH1	2:F:69:GLU:OE2	2.08	0.87
3:O:102:LYS:NZ	3:O:112:ASP:OD1	2.08	0.86
2:H:65:ARG:NH2	2:H:69:GLU:OE1	2.15	0.79
3:M:84:ARG:NH1	2:N:71:ASP:OD2	2.16	0.78
3:O:80:ASN:ND2	3:O:126:TYR:OH	2.21	0.73
1:A:20:ARG:NH1	3:C:107:ASN:OD1	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:8:ILE:HG21	3:I:127:GLN:HB2	1.77	0.66
3:I:38:CYS:SG	3:I:137:ASN:ND2	2.71	0.64
3:E:77:GLU:OE1	2:F:56:THR:HG21	1.99	0.62
1:A:15:TYR:OH	1:A:43:LYS:NZ	2.32	0.62
3:I:20:ARG:NH1	3:K:107:ASN:OD1	2.31	0.62
1:G:107:ASN:OD1	3:O:20:ARG:NH2	2.33	0.62
1:A:17:ARG:NH1	1:A:113:ASP:OD1	2.34	0.61
1:G:55:ASN:O	1:G:59:GLN:OE1	2.19	0.60
2:B:58:LYS:NZ	2:F:75:GLU:O	2.35	0.56
1:A:84:ARG:O	1:A:87:VAL:HG12	2.05	0.56
3:K:58:LEU:HD12	3:K:66:TYR:CZ	2.41	0.55
1:G:102:LYS:HD2	1:G:110:VAL:HG21	1.88	0.55
1:G:17:ARG:NH2	1:G:113:ASP:OD2	2.40	0.55
3:I:17:ARG:NH2	3:I:113:ASP:OD1	2.39	0.55
3:E:34:MET:HE1	3:E:135:GLU:HG2	1.89	0.55
3:E:63:LYS:NZ	3:E:108:GLU:OE1	2.31	0.54
3:M:9:GLU:OE2	3:M:121:ASN:ND2	2.40	0.54
3:O:17:ARG:NH1	3:O:113:ASP:OD1	2.41	0.54
1:G:122:LYS:O	1:G:125:SER:OG	2.25	0.53
1:A:55:ASN:O	1:A:59:GLN:OE1	2.27	0.53
3:M:34:MET:HB3	3:M:134:VAL:CG1	2.39	0.53
1:G:72:LYS:NZ	1:G:118:GLU:OE1	2.39	0.52
3:I:56:PHE:CE1	2:J:59:LEU:HD11	2.45	0.52
3:I:84:ARG:NH1	2:J:71:ASP:OD1	2.43	0.51
2:J:59:LEU:N	2:J:59:LEU:HD12	2.25	0.51
1:G:57:ILE:HG13	1:G:71:VAL:HG22	1.91	0.51
3:M:136:LYS:O	3:M:137:ASN:HB2	2.12	0.50
3:O:136:LYS:O	3:O:137:ASN:HB2	2.11	0.50
3:I:122:LYS:O	3:I:125:SER:OG	2.20	0.50
3:M:26:ASN:ND2	3:O:30:GLU:OE2	2.46	0.49
2:J:53:ASP:OD2	2:J:55:SER:N	2.45	0.48
2:J:55:SER:HA	2:J:58:LYS:HD2	1.95	0.48
2:P:60:SER:OG	2:P:64:LYS:HE3	2.12	0.48
3:I:8:ILE:CG2	3:I:127:GLN:HB2	2.43	0.48
3:M:46:TYR:N	3:M:46:TYR:CD2	2.82	0.48
3:C:82:ASP:OD1	3:C:84:ARG:HG3	2.14	0.48
1:A:19:LEU:HD23	1:A:20:ARG:N	2.29	0.47
3:C:51:ASN:ND2	3:C:101:LYS:HE3	2.29	0.47
3:O:82:ASP:OD1	3:O:84:ARG:HG3	2.15	0.47
3:C:8:ILE:HG21	3:C:127:GLN:HB2	1.97	0.47
1:G:83:PHE:O	1:G:84:ARG:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:84:ARG:O	1:G:87:VAL:HG22	2.15	0.46
1:G:74:ILE:HA	2:H:56:THR:HG23	1.96	0.46
3:E:9:GLU:OE2	3:E:121:ASN:ND2	2.49	0.46
3:O:122:LYS:O	3:O:125:SER:OG	2.30	0.46
3:K:58:LEU:C	3:K:58:LEU:HD23	2.41	0.45
3:C:17:ARG:NH2	3:C:113:ASP:OD2	2.49	0.45
3:M:102:LYS:NZ	3:M:112:ASP:OD1	2.31	0.45
1:G:79:ILE:O	1:G:83:PHE:HB3	2.17	0.45
3:E:67:ASP:OD2	3:E:110:VAL:HG21	2.16	0.45
3:I:67:ASP:CG	3:I:110:VAL:HG21	2.41	0.45
3:E:84:ARG:NH2	2:F:68:ASP:OD2	2.50	0.45
3:I:70:ASP:O	3:I:74:ILE:HD13	2.17	0.45
3:M:136:LYS:O	3:M:137:ASN:CB	2.65	0.45
1:G:111:ASP:OD1	3:O:17:ARG:NH2	2.36	0.44
3:E:72:LYS:HD2	3:E:115:ALA:CB	2.48	0.44
3:M:133:PHE:CD2	3:M:133:PHE:C	2.95	0.44
1:A:61:ASN:ND2	1:A:65:CYS:O	2.46	0.44
3:O:72:LYS:HD3	3:O:115:ALA:HA	1.99	0.44
3:C:20:ARG:HE	3:C:22:GLU:HB2	1.82	0.44
3:I:84:ARG:O	3:I:87:VAL:HG22	2.17	0.44
2:J:72:SER:O	2:J:76:LEU:HG	2.17	0.44
3:K:8:ILE:HG21	3:K:127:GLN:HB2	1.99	0.44
3:O:56:PHE:CD1	2:P:59:LEU:HD21	2.53	0.44
3:E:72:LYS:HE3	3:E:118:GLU:OE1	2.18	0.44
3:E:8:ILE:HG21	3:E:127:GLN:HB2	2.00	0.44
3:E:6:TYR:OH	3:E:131:ILE:HD12	2.18	0.43
1:G:117:ASN:O	1:G:121:ASN:ND2	2.41	0.43
1:G:104:ASP:O	3:O:20:ARG:NE	2.49	0.43
3:I:136:LYS:O	3:I:137:ASN:C	2.61	0.43
1:A:5:ASN:OD1	1:A:5:ASN:N	2.51	0.43
1:G:88:ILE:HG21	1:G:130:ILE:HD11	2.01	0.43
1:A:52:GLU:OE1	2:F:72:SER:OG	2.28	0.43
1:G:82:ASP:OD2	1:G:87:VAL:HG11	2.19	0.43
1:A:17:ARG:NH2	3:C:111:ASP:OD2	2.42	0.43
3:C:24:LEU:HB3	3:C:28:GLU:HG3	2.00	0.43
3:E:84:ARG:O	3:E:87:VAL:HG12	2.19	0.42
3:I:83:PHE:O	3:I:84:ARG:C	2.62	0.42
3:K:75:ILE:O	3:K:79:ILE:HG12	2.19	0.42
3:E:6:TYR:CE1	3:E:131:ILE:CD1	3.02	0.42
1:A:133:PHE:CD2	1:A:133:PHE:C	2.98	0.42
2:P:57:LYS:O	2:P:61:GLU:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:34:MET:HB3	3:M:134:VAL:HG12	2.00	0.42
3:K:117:ASN:O	3:K:121:ASN:ND2	2.52	0.42
3:O:136:LYS:O	3:O:137:ASN:CB	2.67	0.42
1:A:83:PHE:O	1:A:83:PHE:CD2	2.73	0.41
3:C:22:GLU:HG3	3:K:33:ILE:HD12	2.01	0.41
3:I:83:PHE:O	3:I:83:PHE:CG	2.73	0.41
1:G:84:ARG:NH1	2:H:71:ASP:OD2	2.51	0.41
3:M:71:VAL:O	3:M:71:VAL:HG12	2.20	0.41
1:A:48:THR:HG21	2:F:69:GLU:CD	2.46	0.41
3:C:133:PHE:CD2	3:C:133:PHE:C	2.98	0.41
3:I:102:LYS:HG3	3:I:106:ASN:ND2	2.35	0.41
3:I:133:PHE:CD2	3:I:133:PHE:C	2.98	0.41
1:G:49:GLU:OE2	2:H:66:ILE:HG12	2.21	0.41
3:M:29:LEU:O	3:M:33:ILE:HG12	2.21	0.41
3:O:84:ARG:HD3	2:P:71:ASP:OD1	2.21	0.41
1:A:107:ASN:OD1	3:C:20:ARG:HD3	2.21	0.41
3:C:25:ASN:O	3:C:29:LEU:HB2	2.21	0.41
3:E:61:ASN:ND2	3:E:65:CYS:O	2.50	0.41
1:A:88:ILE:HG21	1:A:130:ILE:HD11	2.03	0.41
3:C:79:ILE:HG21	3:C:126:TYR:CE1	2.56	0.41
3:I:128:LYS:HA	3:I:128:LYS:HD2	1.80	0.41
3:M:79:ILE:O	3:M:83:PHE:HB3	2.21	0.41
3:C:128:LYS:HG2	3:C:129:ASP:N	2.32	0.41
3:E:75:ILE:O	3:E:79:ILE:HG12	2.21	0.40
3:M:58:LEU:HD23	3:M:58:LEU:C	2.47	0.40
3:O:8:ILE:HG21	3:O:127:GLN:HB2	2.04	0.40
3:O:58:LEU:C	3:O:58:LEU:HD23	2.46	0.40
3:E:83:PHE:O	3:E:83:PHE:CG	2.73	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	133/150 (89%)	133 (100%)	0	0	100	100
1	G	134/150 (89%)	133 (99%)	1 (1%)	0	100	100
2	B	21/28 (75%)	20 (95%)	1 (5%)	0	100	100
2	D	21/28 (75%)	20 (95%)	1 (5%)	0	100	100
2	F	23/28 (82%)	23 (100%)	0	0	100	100
2	H	22/28 (79%)	22 (100%)	0	0	100	100
2	J	23/28 (82%)	23 (100%)	0	0	100	100
2	L	23/28 (82%)	22 (96%)	1 (4%)	0	100	100
2	N	20/28 (71%)	20 (100%)	0	0	100	100
2	P	19/28 (68%)	18 (95%)	1 (5%)	0	100	100
3	C	136/145 (94%)	135 (99%)	1 (1%)	0	100	100
3	E	131/145 (90%)	130 (99%)	1 (1%)	0	100	100
3	I	131/145 (90%)	130 (99%)	1 (1%)	0	100	100
3	K	132/145 (91%)	132 (100%)	0	0	100	100
3	M	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
3	O	130/145 (90%)	129 (99%)	1 (1%)	0	100	100
All	All	1231/1394 (88%)	1221 (99%)	10 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	133/146 (91%)	133 (100%)	0	100	100
1	G	134/146 (92%)	134 (100%)	0	100	100
2	B	21/26 (81%)	21 (100%)	0	100	100
2	D	21/26 (81%)	21 (100%)	0	100	100
2	F	23/26 (88%)	23 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	22/26 (85%)	22 (100%)	0	100	100
2	J	23/26 (88%)	23 (100%)	0	100	100
2	L	23/26 (88%)	23 (100%)	0	100	100
2	N	20/26 (77%)	20 (100%)	0	100	100
2	P	19/26 (73%)	19 (100%)	0	100	100
3	C	136/143 (95%)	134 (98%)	2 (2%)	57	82
3	E	131/143 (92%)	129 (98%)	2 (2%)	57	82
3	I	131/143 (92%)	130 (99%)	1 (1%)	73	89
3	K	132/143 (92%)	130 (98%)	2 (2%)	57	82
3	M	132/143 (92%)	132 (100%)	0	100	100
3	O	130/143 (91%)	130 (100%)	0	100	100
All	All	1231/1358 (91%)	1224 (99%)	7 (1%)	78	92

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	110	VAL
3	C	128	LYS
3	E	125	SER
3	E	129	ASP
3	I	83	PHE
3	K	125	SER
3	K	138	LYS

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

Mol	Chain	Res	Type
3	C	51	ASN
3	C	55	ASN
3	C	60	ASN
3	C	121	ASN
1	G	60	ASN
1	G	127	GLN
3	I	26	ASN
3	I	137	ASN
2	J	77	GLN
3	K	55	ASN

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Mol	Chain	Res	Type
3	K	59	GLN
3	M	26	ASN
3	O	26	ASN
3	O	55	ASN
3	O	80	ASN

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 oligosaccharides 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	135/150 (90%)	0.14	3 (2%) 62 53	51, 71, 95, 116	0
1	G	135/150 (90%)	0.16	2 (1%) 72 64	48, 69, 94, 106	1 (0%)
2	B	23/28 (82%)	0.49	1 (4%) 40 31	74, 89, 112, 117	0
2	D	23/28 (82%)	0.57	0 100 100	67, 85, 106, 114	0
2	F	25/28 (89%)	0.76	1 (4%) 42 33	73, 90, 114, 122	0
2	H	24/28 (85%)	0.59	2 (8%) 17 14	70, 88, 110, 120	0
2	J	25/28 (89%)	0.43	1 (4%) 42 33	59, 75, 105, 109	0
2	L	25/28 (89%)	0.57	0 100 100	69, 86, 104, 110	0
2	N	22/28 (78%)	0.48	0 100 100	71, 87, 107, 109	0
2	P	21/28 (75%)	0.79	1 (4%) 35 28	73, 92, 100, 105	0
3	C	138/145 (95%)	0.03	1 (0%) 84 79	48, 68, 93, 115	0
3	E	133/145 (91%)	0.15	2 (1%) 72 64	46, 74, 95, 107	0
3	I	133/145 (91%)	0.08	3 (2%) 61 51	38, 62, 84, 100	0
3	K	134/145 (92%)	0.00	1 (0%) 84 79	42, 62, 86, 112	0
3	M	133/145 (91%)	0.16	0 100 100	49, 72, 96, 106	1 (0%)
3	O	132/145 (91%)	0.10	2 (1%) 72 64	51, 74, 95, 103	0
All	All	1261/1394 (90%)	0.18	20 (1%) 70 62	38, 72, 100, 122	2 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	56	THR	3.3
3	C	26	ASN	3.2
2	F	55	SER	2.9
1	A	127	GLN	2.9
1	A	83	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
3	I	126	TYR	2.7
3	I	83	PHE	2.7
3	E	83	PHE	2.6
3	I	137	ASN	2.6
2	H	54	ALA	2.5
2	P	62	CYS	2.5
1	A	139	LYS	2.3
3	K	48	THR	2.3
2	J	59	LEU	2.2
1	G	87	VAL	2.2
3	O	85	PRO	2.2
1	G	50	PHE	2.1
3	E	6	TYR	2.1
2	B	74	MET	2.1
3	O	86	SER	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.