



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:46 PM UTC

PDB ID : 9CB5 / pdb_00009cb5
Title : Crystal structure of nucleolin in complex with MYC promoter G-quadruplex
Authors : Chen, L.; Dickerhoff, J.; Noinaj, N.; Yang, D.
Deposited on : 2024-06-18
Resolution : 2.60 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

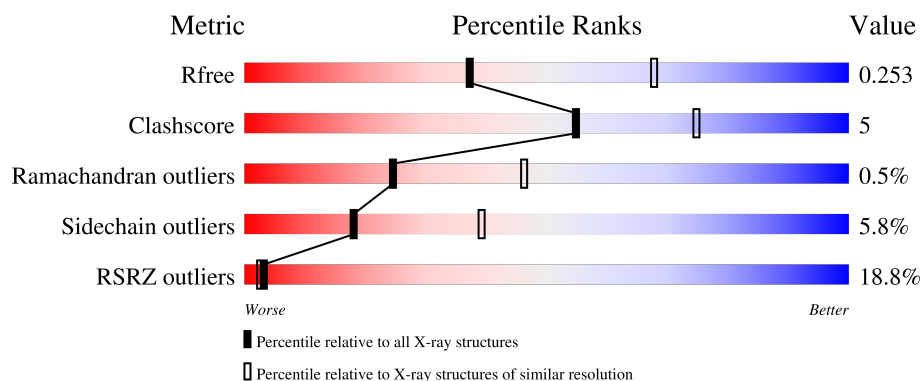
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	347	23% 43% 5% 51%
1	B	347	% 44% 5% 51%
2	C	28	4% 86% 14%
2	F	28	18% 64% 18% 18%
3	D	246	7% 84% 11% 5%

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Mol	Chain	Length	Quality of chain
3	G	246	28% 78% 13% 5%
4	H	215	9% 88% 8%
4	I	215	21% 83% 14%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10339 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 Nucleolin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	0	1	0
			1106	687	201	216	2			
1	B	171	Total	C	N	O	S	0	0	0
			1342	848	225	267	2			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	301	GLY	-	expression tag	UNP P19338
A	302	GLY	-	expression tag	UNP P19338
A	303	GLY	-	expression tag	UNP P19338
A	304	GLY	-	expression tag	UNP P19338
A	305	HIS	-	expression tag	UNP P19338
A	306	MET	-	expression tag	UNP P19338
A	543	SER	CYS	conflict	UNP P19338
B	301	GLY	-	expression tag	UNP P19338
B	302	GLY	-	expression tag	UNP P19338
B	303	GLY	-	expression tag	UNP P19338
B	304	GLY	-	expression tag	UNP P19338
B	305	HIS	-	expression tag	UNP P19338
B	306	MET	-	expression tag	UNP P19338
B	543	SER	CYS	conflict	UNP P19338

- Molecule 2 is a DNA chain called MYC promoter G-quadruplex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	28	Total	C	N	O	P	0	0	0
			585	278	109	171	27			
2	F	23	Total	C	N	O	P	0	0	0
			487	230	91	143	23			

- Molecule 3 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	234	Total	C	N	O	S	0	0	0
			1749	1114	289	340	6			
3	G	233	Total	C	N	O	S	0	0	0
			1712	1089	284	332	7			

- Molecule 4 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	215	Total	C	N	O	S	0	0	0
			1597	994	269	328	6			
4	I	215	Total	C	N	O	S	0	0	0
			1568	972	266	324	6			

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

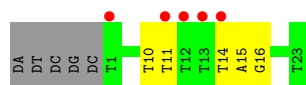
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	2	Total	K	0	0
			2	2		
5	F	2	Total	K	0	0
			2	2		

- Molecule 6 is water.

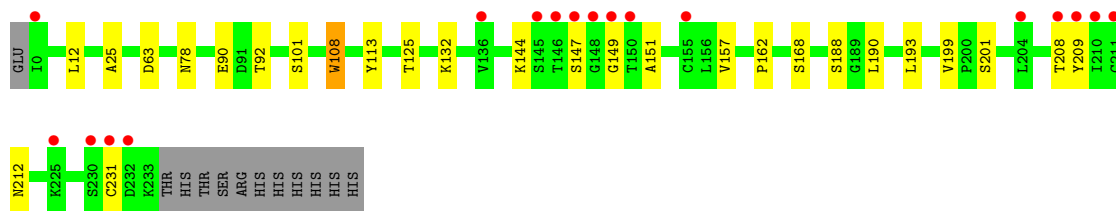
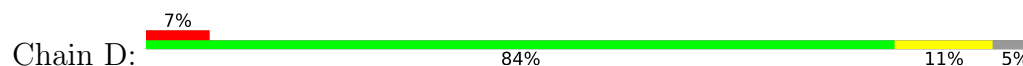
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	7	Total	O	0	0
			7	7		
6	B	34	Total	O	0	0
			34	34		
6	C	12	Total	O	0	0
			12	12		
6	D	35	Total	O	0	0
			35	35		
6	F	5	Total	O	0	0
			5	5		
6	G	21	Total	O	0	0
			21	21		
6	H	55	Total	O	0	0
			55	55		
6	I	20	Total	O	0	0
			20	20		



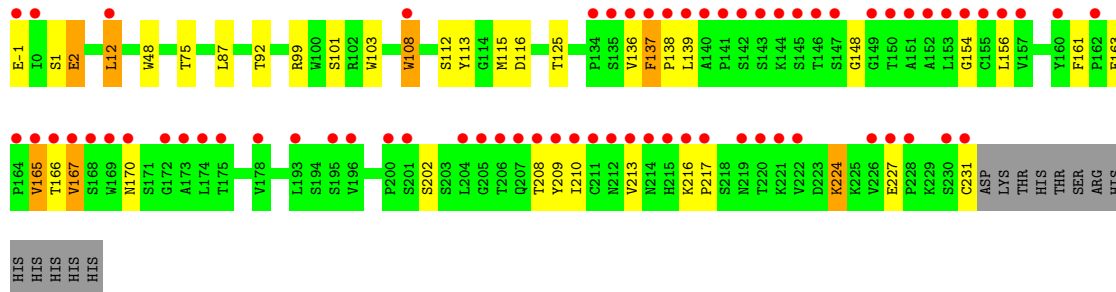
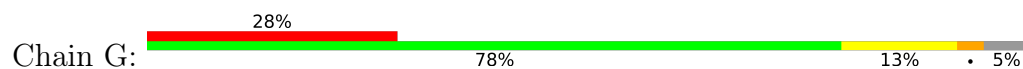
- Molecule 2: MYC promoter G-quadruplex



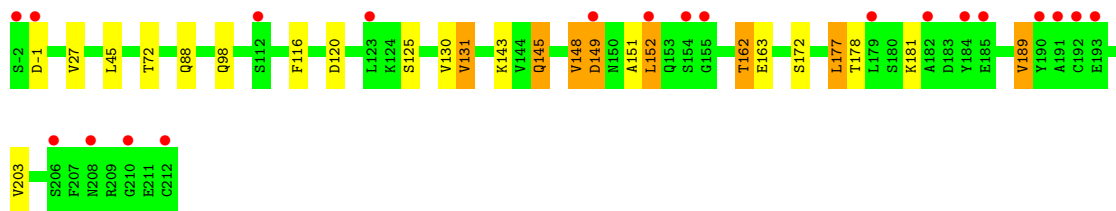
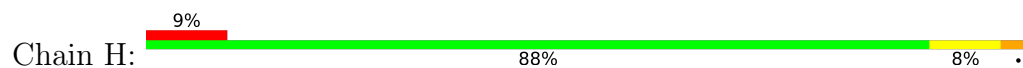
- Molecule 3: Fab heavy chain



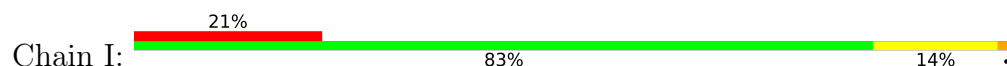
- Molecule 3: Fab heavy chain

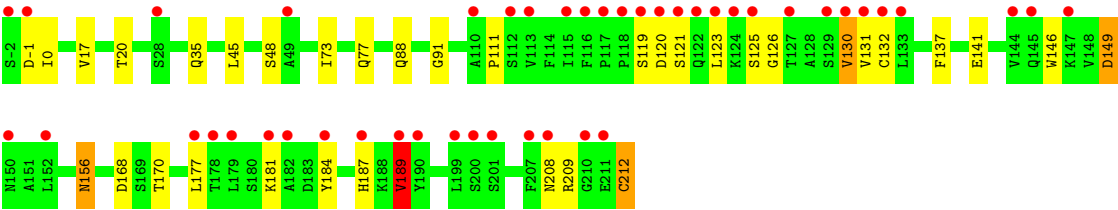


- Molecule 4: Fab light chain



- Molecule 4: Fab light chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.25Å 134.66Å 185.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.43 – 2.60 48.43 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.8 (48.43-2.60) 96.7 (48.43-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.23	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.21.1_5286: ???)	Depositor
R, R_{free}	0.232 , 0.254 0.232 , 0.253	Depositor DCC
R_{free} test set	1999 reflections (3.42%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10339	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
K

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	0.11	0/1117	0.33	0/1514
1	B	0.08	0/1360	0.22	0/1818
2	C	0.16	0/657	0.34	0/1017
2	F	0.19	0/547	0.42	0/847
3	D	0.10	0/1799	0.33	0/2460
3	G	0.13	0/1761	0.35	0/2408
4	H	0.08	0/1630	0.31	0/2216
4	I	0.13	0/1600	0.35	0/2179
All	All	0.12	0/10471	0.33	0/14459

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	1106	0	906	16	0
1	B	1342	0	1342	7	0
2	C	585	0	319	3	0
2	F	487	0	262	6	0
3	D	1749	0	1652	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1712	0	1578	31	0
4	H	1597	0	1532	10	0
4	I	1568	0	1458	21	0
5	C	2	0	0	0	0
5	F	2	0	0	0	0
6	A	7	0	0	0	0
6	B	34	0	0	0	0
6	C	12	0	0	0	0
6	D	35	0	0	0	0
6	F	5	0	0	0	0
6	G	21	0	0	0	0
6	H	55	0	0	0	0
6	I	20	0	0	0	0
All	All	10339	0	9049	92	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 5.

All (92) 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:G:231:CYS:SG	4:I:212:CYS:N	2.46	0.87
1:A:342:ARG:NH2	2:F:10:DT:O4	2.19	0.75
1:A:309:LEU:HD21	1:A:364:LEU:HG	1.72	0.70
1:A:308:ASN:HD21	2:F:10:DT:H3	1.40	0.69
1:A:324:LYS:HA	1:A:341:VAL:HG11	1.75	0.68
3:G:101:SER:HB2	3:G:113:TYR:HB3	1.76	0.67
3:G:101:SER:HA	3:G:116:ASP:HB2	1.77	0.67
3:D:132:LYS:HD3	3:D:190:LEU:HD21	1.78	0.65
4:I:111:PRO:HA	4:I:137:PHE:HB3	1.77	0.64
1:A:309:LEU:HB2	1:A:354:PHE:HE2	1.63	0.63
3:G:138:PRO:HB3	4:I:119:SER:HB2	1.80	0.62
4:H:116:PHE:HB2	4:H:131:VAL:HG23	1.80	0.61
4:I:184:TYR:O	4:I:209:ARG:NH2	2.34	0.60
2:F:15:DA:H2"	2:F:16:DG:C8	2.37	0.59
4:I:130:VAL:HG13	4:I:177:LEU:HB3	1.85	0.59
3:G:216:LYS:HB3	3:G:217:PRO:HD3	1.86	0.58
1:A:339:VAL:HA	3:G:1:SER:HB2	1.86	0.57
3:D:92:THR:HG23	3:D:125:THR:HA	1.86	0.57
1:A:305[A]:HIS:ND1	3:G:75:THR:OG1	2.36	0.54
3:D:147:SER:O	3:D:149:GLY:N	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:GLU:OE2	1:B:467:LYS:NZ	2.39	0.54
1:B:421:LEU:HD23	1:B:432:ALA:HB2	1.90	0.53
4:H:162:THR:HG22	4:H:172:SER:H	1.74	0.53
3:G:99:ARG:NH2	3:G:116:ASP:OD2	2.42	0.53
1:B:309:LEU:HD11	1:B:364:LEU:HG	1.90	0.53
4:H:27:VAL:HG11	4:H:88:GLN:HG3	1.91	0.52
4:I:119:SER:O	4:I:121:SER:N	2.41	0.52
4:H:148:VAL:HG22	4:H:151:ALA:HB3	1.90	0.52
3:G:92:THR:HG23	3:G:125:THR:HA	1.92	0.52
3:D:168:SER:HB3	3:D:212:ASN:HB2	1.92	0.51
3:G:137:PHE:HB2	3:G:138:PRO:HD3	1.93	0.51
1:A:308:ASN:ND2	2:F:10:DT:H3	2.08	0.50
2:F:14:DT:H3	2:F:15:DA:H2	1.59	0.50
4:I:156:ASN:OD1	4:I:156:ASN:N	2.45	0.49
3:G:137:PHE:HB3	4:I:119:SER:HB3	1.94	0.49
4:I:35:GLN:HB2	4:I:45:LEU:HD11	1.93	0.49
4:I:119:SER:C	4:I:121:SER:H	2.21	0.49
3:G:138:PRO:HD3	3:G:156:LEU:HB3	1.96	0.48
3:D:157:VAL:HB	3:D:193:LEU:HB3	1.95	0.48
3:G:231:CYS:HB2	4:I:212:CYS:OXT	2.14	0.48
2:C:2:DA:H2''	2:C:3:DG:C8	2.49	0.47
3:G:137:PHE:CB	3:G:138:PRO:HD3	2.44	0.47
3:G:2:GLU:OE1	3:G:2:GLU:N	2.45	0.47
3:G:167:VAL:HG23	3:G:213:VAL:HA	1.97	0.47
4:I:121:SER:O	4:I:125:SER:N	2.49	0.46
1:B:398:LYS:NZ	2:C:-1:DG:OP2	2.48	0.46
1:B:403:LYS:HA	1:B:403:LYS:HD3	1.71	0.45
3:G:139:LEU:HA	3:G:154:GLY:O	2.15	0.45
4:I:0:ILE:HD12	4:I:91:GLY:HA3	1.98	0.45
4:I:17:VAL:HG22	4:I:73:ILE:HB	1.97	0.45
3:G:48:TRP:HD1	3:G:115:MET:HE1	1.82	0.45
1:A:386:SER:OG	1:A:387:LYS:N	2.49	0.45
3:G:2:GLU:CD	3:G:2:GLU:H	2.22	0.45
1:A:382:LYS:O	2:F:11:DT:H5'	2.17	0.44
3:D:199:VAL:HG21	3:D:209:TYR:CE2	2.53	0.44
3:D:12:LEU:HD11	3:D:162:PRO:HG3	1.99	0.44
3:G:108:TRP:HA	3:G:108:TRP:CE3	2.52	0.44
3:D:144:LYS:H	3:D:144:LYS:HG3	1.60	0.44
1:A:331:PHE:HZ	1:A:378:LEU:HD21	1.82	0.44
3:D:151:ALA:HB2	3:D:201:SER:HA	1.98	0.43
3:D:101:SER:OG	3:D:113:TYR:HB3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:112:SER:OG	4:I:48:SER:OG	2.25	0.43
3:G:170:ASN:HB3	3:G:210:ILE:HG12	2.00	0.43
3:G:138:PRO:CB	4:I:119:SER:HB2	2.47	0.43
1:A:342:ARG:NH1	1:A:353:ASP:OD1	2.52	0.43
1:A:342:ARG:HG2	3:G:103:TRP:CG	2.53	0.43
4:H:125:SER:O	4:H:181:LYS:HD3	2.19	0.43
4:H:145:GLN:HG2	4:H:152:LEU:HD21	2.00	0.43
4:I:168:ASP:OD1	4:I:170:THR:OG1	2.23	0.43
3:G:170:ASN:ND2	3:G:209:TYR:H	2.15	0.43
4:I:132:CYS:HB2	4:I:146:TRP:CH2	2.54	0.43
1:B:309:LEU:HD13	1:B:360:LEU:HG	2.00	0.43
4:I:126:GLY:HA2	4:I:181:LYS:HE2	2.00	0.43
1:A:398:LYS:HA	1:A:432:ALA:H	1.83	0.42
1:A:309:LEU:HD13	1:A:360:LEU:HD11	2.01	0.42
4:H:162:THR:HG23	4:H:163:GLU:O	2.18	0.42
3:G:148:GLY:HA2	3:G:202:SER:N	2.35	0.42
4:H:130:VAL:HB	4:H:177:LEU:HB3	2.02	0.42
3:D:188:SER:C	3:D:190:LEU:H	2.28	0.42
3:D:108:TRP:HA	3:D:108:TRP:CE3	2.55	0.42
4:I:149:ASP:HA	4:I:189:VAL:HG12	2.02	0.41
3:D:25:ALA:O	3:D:78:ASN:ND2	2.51	0.41
1:A:309:LEU:HD12	1:A:309:LEU:HA	1.87	0.41
1:B:381:PRO:HB2	2:C:10:DT:C2	2.56	0.41
3:G:170:ASN:N	3:G:210:ILE:O	2.53	0.41
3:G:108:TRP:HA	3:G:108:TRP:HE3	1.85	0.41
3:G:165:VAL:O	3:G:166:THR:C	2.64	0.41
3:G:224:LYS:HE2	3:G:224:LYS:HB3	1.64	0.41
4:H:149:ASP:HA	4:H:189:VAL:HG13	2.01	0.41
4:I:123:LEU:O	4:I:181:LYS:NZ	2.53	0.41
3:G:12:LEU:HD11	3:G:161:PHE:HE2	1.85	0.40
4:H:98:GLN:OE1	4:H:98:GLN:N	2.46	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	168/347 (48%)	147 (88%)	20 (12%)	1 (1%)	21	42
1	B	169/347 (49%)	168 (99%)	1 (1%)	0	100	100
3	D	232/246 (94%)	219 (94%)	12 (5%)	1 (0%)	30	51
3	G	231/246 (94%)	208 (90%)	21 (9%)	2 (1%)	14	30
4	H	213/215 (99%)	201 (94%)	11 (5%)	1 (0%)	24	46
4	I	213/215 (99%)	193 (91%)	19 (9%)	1 (0%)	24	46
All	All	1226/1616 (76%)	1136 (93%)	84 (7%)	6 (0%)	24	46

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	401	PRO
3	D	231	CYS
3	G	137	PHE
3	G	208	THR
4	H	149	ASP
4	I	189	VAL

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	78/289 (27%)	75 (96%)	3 (4%)	29	56
1	B	142/289 (49%)	134 (94%)	8 (6%)	19	40
3	D	185/208 (89%)	181 (98%)	4 (2%)	45	72
3	G	174/208 (84%)	163 (94%)	11 (6%)	16	36
4	H	180/187 (96%)	166 (92%)	14 (8%)	11	26
4	I	169/187 (90%)	155 (92%)	14 (8%)	10	23
All	All	928/1368 (68%)	874 (94%)	54 (6%)	18	39

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	309	LEU
1	A	339	VAL
1	A	391	ASP
1	B	339	VAL
1	B	361	GLU
1	B	371	VAL
1	B	377	LYS
1	B	393	ARG
1	B	406	GLN
1	B	429	LYS
1	B	459	ILE
3	D	63	ASP
3	D	90	GLU
3	D	108	TRP
3	D	208	THR
3	G	-1	GLU
3	G	2	GLU
3	G	12	LEU
3	G	87	LEU
3	G	108	TRP
3	G	136	VAL
3	G	163	GLU
3	G	165	VAL
3	G	167	VAL
3	G	224	LYS
3	G	227	GLU
4	H	-1	ASP
4	H	45	LEU
4	H	72	THR
4	H	120	ASP
4	H	131	VAL
4	H	143	LYS
4	H	145	GLN
4	H	148	VAL
4	H	152	LEU
4	H	162	THR
4	H	177	LEU
4	H	178	THR
4	H	189	VAL
4	H	203	VAL
4	I	-1	ASP
4	I	20	THR

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Mol	Chain	Res	Type
4	I	77	GLN
4	I	88	GLN
4	I	120	ASP
4	I	130	VAL
4	I	131	VAL
4	I	141	GLU
4	I	149	ASP
4	I	156	ASN
4	I	187	HIS
4	I	189	VAL
4	I	208	ASN
4	I	212	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	179	HIS
3	G	14	GLN
3	G	83	GLN
4	H	122	GLN
4	H	135	ASN
4	H	150	ASN
4	I	88	GLN

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](#)

Of 4 ligands modelled in this entry, 4 are 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 [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	169/347 (48%)	1.87	80 (47%) 0 0	31, 106, 144, 151	1 (0%)
1	B	171/347 (49%)	0.20	4 (2%) 61 55	33, 49, 72, 83	0
2	C	28/28 (100%)	0.16	1 (3%) 46 40	35, 48, 70, 112	0
2	F	23/28 (82%)	0.83	5 (21%) 2 2	51, 60, 128, 148	0
3	D	234/246 (95%)	0.56	18 (7%) 19 15	30, 50, 111, 134	0
3	G	233/246 (94%)	1.18	69 (29%) 1 1	38, 62, 140, 153	0
4	H	215/215 (100%)	0.40	20 (9%) 14 11	30, 47, 95, 119	0
4	I	215/215 (100%)	1.07	45 (20%) 2 2	39, 70, 127, 153	0
All	All	1288/1672 (77%)	0.85	242 (18%) 3 2	30, 58, 134, 153	1 (0%)

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	-4	DA	6.2
3	D	145	SER	5.9
3	G	209	TYR	5.7
3	G	138	PRO	5.6
1	A	465	GLY	5.4
1	A	458	SER	5.3
1	A	433	TYR	5.3
1	A	425	ASP	5.3
1	A	470	ASN	5.2
1	A	460	SER	5.0
1	A	427	LYS	5.0
1	A	423	SER	4.9
1	A	469	GLN	4.9
3	G	140	ALA	4.8
1	A	455	ASP	4.8
4	I	118	PRO	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	428	SER	4.8
1	A	397	ALA	4.7
1	A	459	ILE	4.7
1	A	402	TYR	4.7
3	G	222	VAL	4.7
1	A	464	THR	4.6
1	A	405	THR	4.6
4	I	117	PRO	4.6
1	A	441	ASP	4.6
3	G	153	LEU	4.5
1	A	400	LEU	4.5
3	G	217	PRO	4.4
3	G	220	THR	4.4
4	I	127	THR	4.4
1	A	424	LYS	4.2
4	I	131	VAL	4.2
3	D	0	ILE	4.2
3	G	0	ILE	4.2
3	G	139	LEU	4.1
1	A	415	ASP	4.1
1	A	466	GLU	4.1
3	D	225	LYS	4.1
1	A	431	ILE	4.1
1	A	462	TYR	4.1
1	A	392	ALA	4.0
1	B	472	ASP	4.0
3	G	195	SER	4.0
3	G	152	ALA	4.0
3	D	209	TYR	4.0
4	I	120	ASP	4.0
1	A	461	LEU	4.0
1	A	447	GLU	3.9
1	A	414	GLU	3.9
3	G	172	GLY	3.9
3	D	232	ASP	3.9
1	A	452	THR	3.8
3	G	208	THR	3.8
1	A	443	GLU	3.8
4	I	189	VAL	3.8
3	D	231	CYS	3.8
1	A	463	TYR	3.8
4	I	-2	SER	3.8

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Mol	Chain	Res	Type	RSRZ
4	I	207	PHE	3.8
3	D	146	THR	3.7
4	I	129	SER	3.7
4	I	211	GLU	3.7
3	D	147	SER	3.7
1	A	438	THR	3.6
3	G	219	ASN	3.6
1	A	457	ARG	3.6
1	A	456	GLY	3.6
4	I	122	GLN	3.6
3	G	146	THR	3.5
1	A	399	ASN	3.5
3	D	148	GLY	3.5
1	A	439	GLU	3.5
3	G	149	GLY	3.5
4	I	116	PHE	3.5
1	A	416	ALA	3.5
3	G	108	TRP	3.5
1	A	403	LYS	3.4
3	G	165	VAL	3.4
1	A	440	ALA	3.4
3	G	151	ALA	3.4
1	A	341	VAL	3.4
3	G	166	THR	3.4
1	A	446	PHE	3.4
1	A	430	GLY	3.3
3	G	231	CYS	3.3
3	G	142	SER	3.3
1	A	412	VAL	3.3
4	I	178	THR	3.3
1	A	454	ILE	3.3
3	G	230	SER	3.2
3	G	164	PRO	3.2
3	D	149	GLY	3.2
4	I	184	TYR	3.2
4	H	149	ASP	3.2
1	A	302	GLY	3.2
1	A	407	ASP	3.2
3	G	204	LEU	3.2
2	F	12	DT	3.1
3	G	150	THR	3.1
3	G	137	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
3	G	212	ASN	3.1
3	G	145	SER	3.1
3	G	200	PRO	3.1
3	D	150	THR	3.1
3	G	210	ILE	3.1
1	A	429	LYS	3.1
4	I	123	LEU	3.1
1	B	425	ASP	3.1
3	G	207	GLN	3.1
4	H	182	ALA	3.1
2	F	1	DT	3.1
3	G	-1	GLU	3.0
1	A	437	LYS	3.0
1	A	426	GLY	3.0
1	A	434	ILE	3.0
1	A	394	THR	3.0
3	G	173	ALA	3.0
3	G	213	VAL	3.0
1	A	395	LEU	3.0
2	F	11	DT	3.0
1	A	436	PHE	3.0
3	G	167	VAL	3.0
1	A	411	GLU	2.9
4	H	112	SER	2.9
1	A	442	ALA	2.9
1	A	453	GLU	2.9
2	F	14	DT	2.9
3	G	221	LYS	2.9
3	G	134	PRO	2.9
3	G	155	CYS	2.9
3	G	156	LEU	2.9
3	G	174	LEU	2.9
1	A	435	GLU	2.8
3	G	175	THR	2.8
3	D	230	SER	2.8
3	G	135	SER	2.8
1	A	449	LYS	2.8
3	G	206	THR	2.8
2	F	13	DT	2.8
3	G	169	TRP	2.8
1	A	384	LYS	2.8
1	A	404	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	422	VAL	2.8
3	G	227	GLU	2.8
4	H	190	TYR	2.8
3	G	201	SER	2.7
4	I	113	VAL	2.7
3	G	160	TYR	2.7
4	I	132	CYS	2.7
3	G	214	ASN	2.7
1	A	420	ARG	2.7
1	A	398	LYS	2.7
1	A	444	LYS	2.7
3	G	170	ASN	2.7
3	G	168	SER	2.7
4	H	-2	SER	2.7
3	G	228	PRO	2.7
4	H	179	LEU	2.6
3	G	144	LYS	2.6
3	G	193	LEU	2.6
1	A	383	GLY	2.6
3	D	136	VAL	2.6
3	G	147	SER	2.6
4	I	125	SER	2.6
4	H	208	ASN	2.6
4	I	190	TYR	2.6
3	G	136	VAL	2.6
4	I	119	SER	2.5
4	I	208	ASN	2.5
3	D	210	ILE	2.5
1	A	396	LEU	2.5
4	H	191	ALA	2.5
4	I	182	ALA	2.5
4	I	152	LEU	2.5
1	A	401	PRO	2.5
4	I	124	LYS	2.4
4	I	130	VAL	2.4
3	G	12	LEU	2.4
4	I	201	SER	2.4
1	A	417	ALA	2.4
4	I	115	ILE	2.4
3	G	205	GLY	2.4
4	I	199	LEU	2.4
3	D	208	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	382	LYS	2.4
3	G	141	PRO	2.4
3	G	162	PRO	2.4
3	G	154	GLY	2.4
4	I	210	GLY	2.4
4	I	145	GLN	2.4
1	A	419	ILE	2.3
1	A	385	ASP	2.3
1	A	451	GLY	2.3
1	A	468	GLY	2.3
4	I	187	HIS	2.3
1	B	302	GLY	2.3
4	H	212	CYS	2.3
3	G	178	VAL	2.3
4	I	144	VAL	2.3
3	G	157	VAL	2.3
1	A	432	ALA	2.3
1	A	445	THR	2.3
1	A	303	GLY	2.3
3	D	211	CYS	2.2
4	H	154	SER	2.2
4	I	179	LEU	2.2
1	A	388	LYS	2.2
4	I	110	ALA	2.2
4	H	185	GLU	2.2
4	H	152	LEU	2.2
3	G	216	LYS	2.2
4	I	147	LYS	2.2
3	G	215	HIS	2.2
3	D	155	CYS	2.2
4	I	181	LYS	2.2
3	G	226	VAL	2.2
3	D	204	LEU	2.2
3	G	143	SER	2.2
3	G	211	CYS	2.1
4	H	184	TYR	2.1
3	G	196	VAL	2.1
4	I	-1	ASP	2.1
1	A	413	PHE	2.1
4	I	121	SER	2.1
4	I	49	ALA	2.1
1	A	450	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
4	I	133	LEU	2.1
4	I	177	LEU	2.1
4	H	192	CYS	2.1
4	H	155	GLY	2.1
4	H	210	GLY	2.1
4	H	206	SER	2.1
4	I	28	SER	2.1
1	B	471	GLN	2.1
1	A	421	LEU	2.1
4	H	123	LEU	2.1
4	I	200	SER	2.0
4	I	150	ASN	2.0
4	H	-1	ASP	2.0
4	H	193	GLU	2.0
4	I	112	SER	2.0
1	A	409	LEU	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](#)

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. 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	B-factors($\text{\AA}^2$)	Q<0.9
5	K	F	101	1/1	0.91	0.06	56,56,56,56	0
5	K	F	102	1/1	0.97	0.03	41,41,41,41	0
5	K	C	101	1/1	0.99	0.02	35,35,35,35	0
5	K	C	102	1/1	0.99	0.05	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.