



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:28 AM UTC

PDB ID : 2XMQ / pdb_00002xmQ
Title : Crystal structure of human NDRG2 protein provides insight into its role as a tumor suppressor
Authors : Hwang, J.; Kim, Y.; Lee, H.; Kim, M.H.
Deposited on : 2010-07-29
Resolution : 2.81 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
Mogul : 2022.3.0, CSD as543be (2022)
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

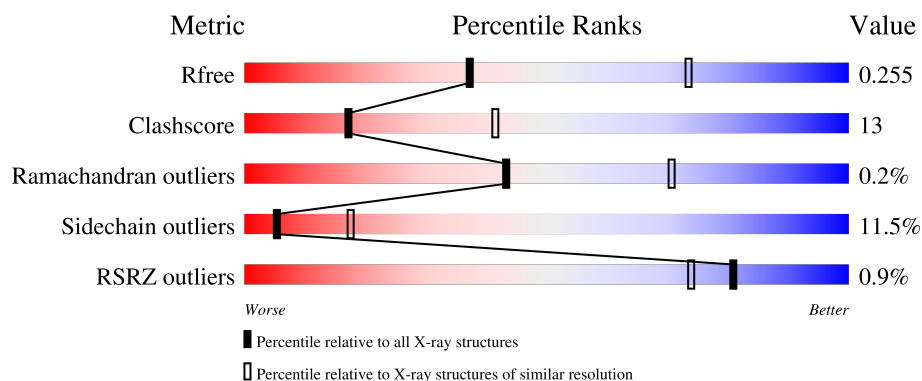
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	281	62%32% . .
1	B	281	67%27%6% .
1	C	281	64%29%5% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6720 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.

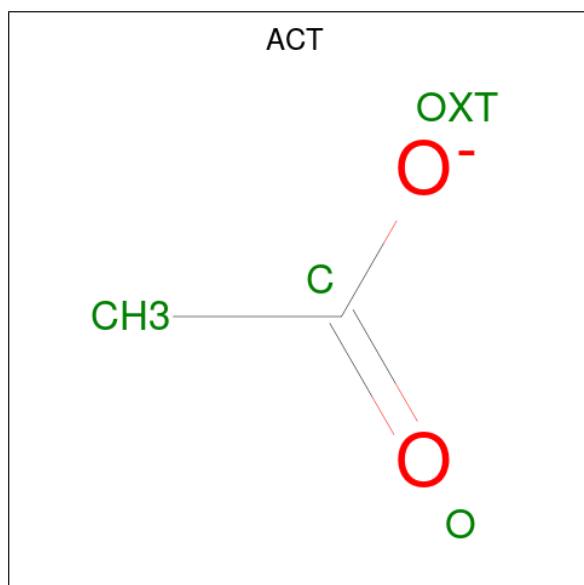
- Molecule 1 is a protein called PROTEIN NDRG2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2205	1409	366	417	13			
1	B	281	Total	C	N	O	S	0	0	0
			2205	1409	366	417	13			
1	C	281	Total	C	N	O	S	0	0	0
			2205	1409	366	417	13			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	218	ASN	LEU	conflict	UNP Q9UN36
B	218	ASN	LEU	conflict	UNP Q9UN36
C	218	ASN	LEU	conflict	UNP Q9UN36

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0

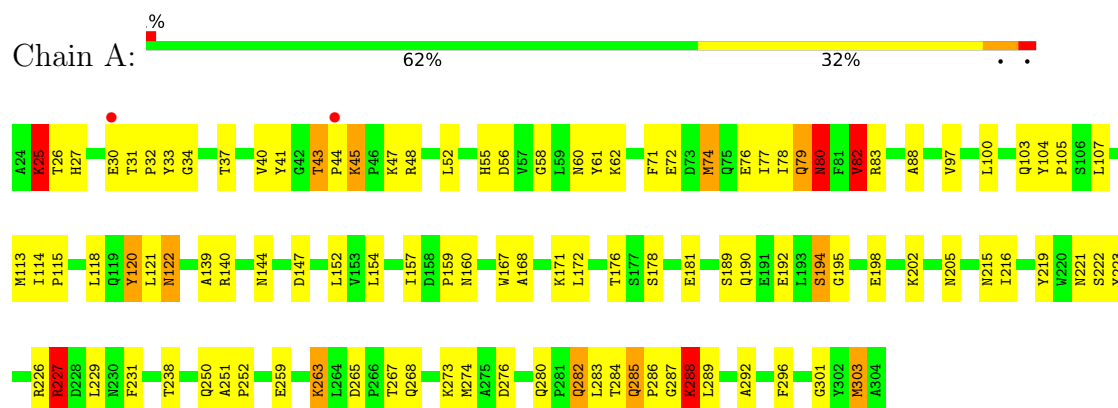
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	36	Total O 36 36	0	0
3	B	23	Total O 23 23	0	0
3	C	34	Total O 34 34	0	0

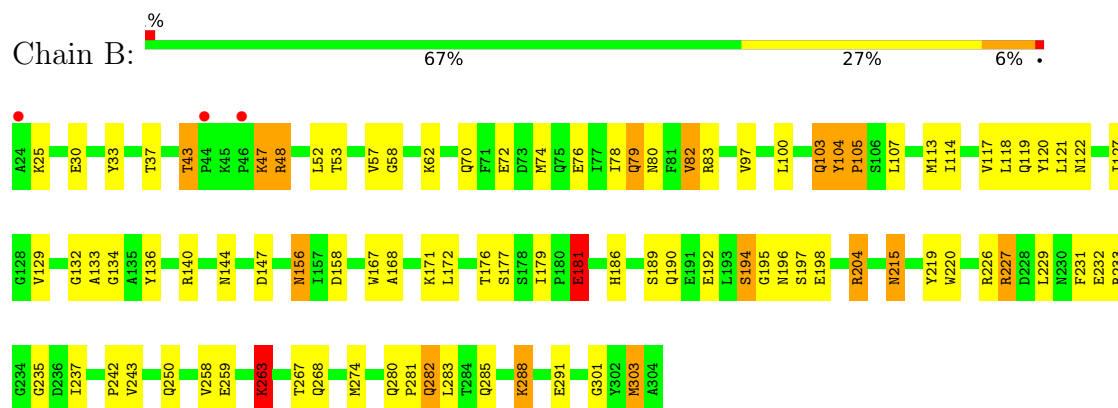
3 Residue-property plots

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.

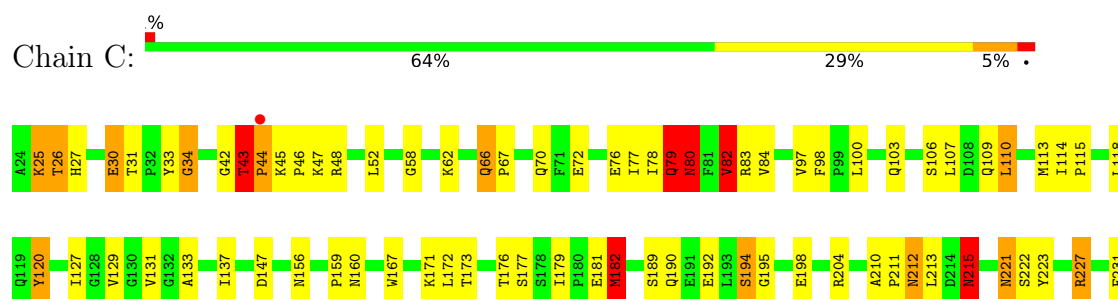
• Molecule 1: PROTEIN NDRG2



• Molecule 1: PROTEIN NDRG2



• Molecule 1: PROTEIN NDRG2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.41Å 88.90Å 126.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.81 40.00 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.2 (40.00-2.81) 99.3 (40.00-2.81)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.93 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.201 , 0.258 0.201 , 0.255	Depositor DCC
R_{free} test set	1242 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 27.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6720	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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

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

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	1.60	21/2263 (0.9%)	1.49	25/3080 (0.8%)
1	B	1.59	18/2263 (0.8%)	1.44	20/3080 (0.6%)
1	C	1.62	17/2263 (0.8%)	1.53	31/3080 (1.0%)
All	All	1.60	56/6789 (0.8%)	1.49	76/9240 (0.8%)

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	B	0	1
1	C	0	2
All	All	0	3

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	114	ILE	CA-CB	-12.59	1.47	1.54
1	B	30	GLU	CA-C	-9.25	1.41	1.52
1	A	168	ALA	CA-CB	-9.01	1.39	1.53
1	C	212	ASN	CG-OD1	-8.10	1.08	1.23
1	C	30	GLU	N-CA	-7.92	1.36	1.45
1	A	103	GLN	CB-CG	-7.85	1.28	1.52
1	C	292	ALA	CA-CB	-7.84	1.41	1.53
1	A	30	GLU	CA-C	-7.43	1.43	1.52
1	C	204	ARG	CZ-NH1	-7.39	1.22	1.32
1	C	212	ASN	CB-CG	-7.20	1.34	1.52
1	B	179	ILE	CA-C	7.17	1.59	1.52
1	C	30	GLU	CA-C	-6.93	1.44	1.52
1	B	179	ILE	CA-CB	-6.89	1.50	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	268	GLN	CD-OE1	-6.78	1.10	1.23
1	A	144	ASN	CG-ND2	-6.71	1.19	1.33
1	B	291	GLU	C-O	-6.45	1.16	1.24
1	B	168	ALA	CA-CB	-6.44	1.43	1.53
1	C	131	VAL	CA-CB	6.17	1.62	1.54
1	A	41	TYR	CA-C	-6.16	1.44	1.52
1	C	70	GLN	CD-OE1	-6.01	1.12	1.23
1	C	129	VAL	C-O	-5.97	1.17	1.24
1	B	267	THR	CA-CB	5.92	1.63	1.53
1	B	237	ILE	CA-CB	5.86	1.61	1.53
1	B	282	GLN	CD-OE1	-5.76	1.12	1.23
1	C	84	VAL	C-O	-5.72	1.18	1.24
1	A	45	LYS	N-CA	-5.66	1.41	1.46
1	C	110	LEU	C-O	-5.65	1.17	1.24
1	A	285	GLN	CD-OE1	-5.64	1.12	1.23
1	C	156	ASN	CG-ND2	-5.61	1.21	1.33
1	A	292	ALA	CA-CB	-5.52	1.44	1.53
1	C	215	ASN	CG-ND2	-5.49	1.21	1.33
1	C	221	ASN	CG-ND2	-5.49	1.21	1.33
1	C	250	GLN	CG-CD	5.47	1.65	1.52
1	B	168	ALA	C-O	-5.45	1.17	1.24
1	A	288	LYS	CA-C	5.42	1.59	1.52
1	B	47	LYS	CA-C	5.33	1.60	1.52
1	B	119	GLN	C-O	-5.32	1.17	1.24
1	C	179	ILE	N-CA	-5.30	1.40	1.46
1	A	120	TYR	CG-CD1	-5.28	1.28	1.39
1	A	120	TYR	CE2-CZ	-5.28	1.25	1.38
1	A	139	ALA	CA-CB	-5.24	1.45	1.53
1	A	285	GLN	CG-CD	-5.23	1.39	1.52
1	A	120	TYR	CE1-CZ	-5.23	1.25	1.38
1	C	250	GLN	CB-CG	5.21	1.68	1.52
1	B	258	VAL	N-CA	5.21	1.52	1.46
1	A	152	LEU	C-O	-5.16	1.18	1.24
1	A	120	TYR	CG-CD2	-5.15	1.28	1.39
1	A	296	PHE	C-O	-5.15	1.18	1.24
1	B	243	VAL	CA-C	-5.10	1.46	1.52
1	A	30	GLU	CD-OE2	5.09	1.35	1.25
1	A	227	ARG	NE-CZ	5.09	1.38	1.33
1	B	156	ASN	CG-ND2	-5.08	1.22	1.33
1	B	136	TYR	C-O	-5.07	1.18	1.24
1	B	70	GLN	N-CA	5.04	1.52	1.45
1	A	40	VAL	CA-CB	5.03	1.60	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	127	ILE	CA-CB	-5.03	1.48	1.54

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	43	THR	N-CA-C	-12.44	95.39	110.31
1	A	43	THR	CA-C-N	-9.85	110.76	120.21
1	A	43	THR	C-N-CA	-9.85	110.76	120.21
1	C	212	ASN	N-CA-CB	-9.63	96.07	110.61
1	B	43	THR	N-CA-C	-9.47	97.99	110.40
1	A	285	GLN	CA-CB-CG	-9.30	95.50	114.10
1	A	43	THR	N-CA-C	-9.21	98.34	110.40
1	C	204	ARG	NE-CZ-NH2	8.88	127.19	119.20
1	A	82	VAL	CB-CA-C	-8.68	99.65	111.63
1	B	43	THR	CA-C-N	-8.59	109.11	119.84
1	B	43	THR	C-N-CA	-8.59	109.11	119.84
1	B	30	GLU	CA-CB-CG	-8.58	96.94	114.10
1	C	182	MET	CB-CG-SD	8.18	137.24	112.70
1	C	212	ASN	CB-CG-ND2	7.72	127.98	116.40
1	C	181	GLU	N-CA-C	-7.68	102.91	111.28
1	A	30	GLU	CA-CB-CG	-7.52	99.06	114.10
1	C	30	GLU	CA-CB-CG	-7.42	99.26	114.10
1	C	43	THR	CA-C-N	-7.28	110.75	119.84
1	C	43	THR	C-N-CA	-7.28	110.75	119.84
1	C	82	VAL	CB-CA-C	-7.12	101.81	111.63
1	A	74	MET	N-CA-C	-7.07	103.00	111.69
1	B	82	VAL	CB-CA-C	-6.95	101.33	111.68
1	A	34	GLY	N-CA-C	-6.94	101.87	112.84
1	B	204	ARG	NE-CZ-NH2	6.83	125.35	119.20
1	C	66	GLN	CA-C-N	-6.77	112.20	119.24
1	C	66	GLN	C-N-CA	-6.77	112.20	119.24
1	B	186	HIS	N-CA-C	-6.59	104.26	112.90
1	C	103	GLN	CB-CA-C	-6.58	100.68	111.68
1	C	213	LEU	N-CA-C	6.55	119.26	111.33
1	C	58	GLY	N-CA-C	-6.42	106.28	114.37
1	C	80	ASN	N-CA-C	-6.42	103.75	113.89
1	C	80	ASN	CA-CB-CG	-6.35	106.25	112.60
1	C	127	ILE	N-CA-C	-6.35	98.59	107.80
1	C	212	ASN	CB-CG-OD1	-6.35	108.11	120.80
1	A	25	LYS	N-CA-C	6.31	118.57	108.41
1	A	122	ASN	CB-CA-C	-6.17	101.75	111.51
1	B	105	PRO	CB-CA-C	-6.03	103.52	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	181	GLU	CG-CD-OE1	6.02	132.24	118.40
1	C	182	MET	CG-SD-CE	-5.97	87.76	100.90
1	B	117	VAL	N-CA-C	-5.96	104.93	110.53
1	A	219	TYR	N-CA-C	-5.90	104.43	111.69
1	A	103	GLN	N-CA-CB	-5.86	96.03	110.32
1	C	289	LEU	N-CA-C	-5.86	104.97	111.36
1	A	122	ASN	N-CA-C	5.82	119.69	112.24
1	A	77	ILE	CB-CA-C	-5.78	104.25	112.22
1	B	58	GLY	N-CA-C	-5.78	107.03	113.79
1	A	178	SER	N-CA-C	-5.77	103.32	110.41
1	B	220	TRP	N-CA-C	-5.72	105.12	111.36
1	B	263	LYS	CB-CG-CD	5.71	124.42	111.30
1	B	219	TYR	N-CA-C	-5.61	105.16	112.23
1	C	211	PRO	CA-C-N	5.60	131.16	122.49
1	C	211	PRO	C-N-CA	5.60	131.16	122.49
1	C	212	ASN	N-CA-C	-5.58	105.83	113.30
1	C	26	THR	N-CA-C	5.50	118.22	109.96
1	A	227	ARG	CG-CD-NE	5.42	123.92	112.00
1	A	289	LEU	N-CA-C	-5.39	105.49	111.36
1	A	34	GLY	CA-C-N	-5.30	113.59	122.92
1	A	34	GLY	C-N-CA	-5.30	113.59	122.92
1	C	80	ASN	N-CA-CB	5.28	118.55	110.95
1	C	42	GLY	N-CA-C	-5.27	106.03	112.68
1	C	77	ILE	CB-CA-C	-5.25	104.98	112.22
1	A	103	GLN	CB-CA-C	5.20	119.41	111.76
1	A	77	ILE	N-CA-C	5.18	115.95	110.72
1	C	43	THR	CB-CA-C	5.17	117.72	109.96
1	C	25	LYS	N-CA-C	5.14	116.69	108.41
1	A	227	ARG	CD-NE-CZ	5.13	131.58	124.40
1	A	276	ASP	N-CA-C	5.13	118.80	112.24
1	B	57	VAL	CB-CA-C	-5.11	103.71	111.33
1	C	34	GLY	N-CA-C	-5.10	104.54	112.45
1	B	144	ASN	N-CA-C	5.07	117.70	111.82
1	B	104	TYR	CA-C-N	5.07	125.00	119.78
1	B	104	TYR	C-N-CA	5.07	125.00	119.78
1	A	80	ASN	N-CA-C	5.05	119.09	113.02
1	A	227	ARG	CB-CG-CD	5.05	122.92	111.30
1	B	281	PRO	CB-CA-C	-5.04	104.35	112.21
1	B	103	GLN	CB-CA-C	-5.02	102.88	111.31

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	233	ARG	Peptide
1	C	44	PRO	Peptide
1	C	79	GLN	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	2205	0	2142	61	0
1	B	2205	0	2142	51	0
1	C	2205	0	2142	59	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
2	C	4	0	3	0	0
3	A	36	0	0	3	0
3	B	23	0	0	2	0
3	C	34	0	0	0	0
All	All	6720	0	6435	165	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 13.

All (165) 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:B:79:GLN:NE2	1:B:79:GLN:HA	1.72	1.00
1:A:79:GLN:NE2	1:A:79:GLN:HA	1.77	0.99
1:B:79:GLN:HA	1:B:79:GLN:HE21	1.26	0.99
1:C:167:TRP:O	1:C:171:LYS:HG3	1.62	0.98
1:A:79:GLN:HA	1:A:79:GLN:HE21	1.32	0.94
1:A:227:ARG:HH11	1:A:227:ARG:HB3	1.34	0.91
1:C:79:GLN:NE2	1:C:79:GLN:HA	1.85	0.89
1:A:282:GLN:HE21	1:A:282:GLN:H	1.21	0.88
1:B:231:PHE:O	1:B:263:LYS:HG2	1.75	0.87
1:A:55:HIS:HE1	1:A:88:ALA:H	1.22	0.85
1:C:303:MET:HE3	1:C:303:MET:HA	1.56	0.84
1:B:280:GLN:NE2	1:B:282:GLN:HE22	1.78	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:SER:OG	1:C:192:GLU:HG3	1.80	0.79
1:A:227:ARG:HH11	1:A:227:ARG:CB	1.95	0.78
1:C:79:GLN:HA	1:C:79:GLN:HE21	1.47	0.75
1:A:55:HIS:CE1	1:A:88:ALA:H	2.06	0.72
1:B:181:GLU:OE1	1:B:204:ARG:NH1	2.26	0.69
1:A:282:GLN:H	1:A:282:GLN:NE2	1.91	0.69
1:C:173:THR:HG22	1:C:182:MET:HE1	1.75	0.69
1:A:303:MET:SD	1:B:303:MET:HE3	2.34	0.68
1:C:177:SER:HB2	1:C:182:MET:HE3	1.75	0.67
1:B:189:SER:OG	1:B:192:GLU:HG3	1.95	0.67
1:C:26:THR:O	1:C:27:HIS:HD2	1.78	0.67
1:C:106:SER:OG	1:C:109:GLN:HG3	1.96	0.66
1:C:45:LYS:HG3	1:C:80:ASN:O	1.97	0.64
1:A:167:TRP:O	1:A:171:LYS:HG3	1.98	0.63
1:C:177:SER:HB2	1:C:182:MET:CE	2.28	0.62
1:B:74:MET:O	1:B:78:ILE:HG12	2.00	0.62
1:B:167:TRP:O	1:B:171:LYS:HG3	2.00	0.61
1:A:301:GLY:HA3	1:B:48:ARG:NH2	2.16	0.61
1:C:303:MET:HA	1:C:303:MET:CE	2.26	0.60
1:A:231:PHE:O	1:A:263:LYS:HD3	2.01	0.59
1:C:177:SER:CB	1:C:182:MET:HE3	2.32	0.59
1:C:97:VAL:HA	1:C:215:ASN:HD21	1.66	0.59
1:B:280:GLN:HB3	1:B:283:LEU:HD12	1.84	0.59
1:A:303:MET:HE3	1:B:303:MET:SD	2.43	0.59
1:A:303:MET:HE3	1:A:303:MET:HA	1.85	0.58
1:A:284:THR:C	1:A:285:GLN:HG3	2.28	0.58
1:C:167:TRP:O	1:C:171:LYS:CG	2.46	0.57
1:C:227:ARG:HB2	1:C:227:ARG:HH11	1.69	0.57
1:A:189:SER:OG	1:A:192:GLU:HG3	2.05	0.57
1:C:280:GLN:HB3	1:C:283:LEU:HD12	1.86	0.57
1:A:74:MET:O	1:A:78:ILE:HG12	2.04	0.57
1:B:83:ARG:N	1:B:83:ARG:HD3	2.21	0.56
1:C:110:LEU:HD23	1:C:113:MET:HE3	1.87	0.56
1:A:83:ARG:N	1:A:83:ARG:HD3	2.21	0.56
1:B:226:ARG:HH11	1:B:226:ARG:HG2	1.70	0.56
1:B:274:MET:HE1	1:B:285:GLN:HB2	1.87	0.56
1:B:132:GLY:O	1:B:133:ALA:C	2.46	0.56
1:C:212:ASN:OD1	1:C:212:ASN:C	2.43	0.56
1:C:274:MET:HE3	1:C:288:LYS:HB3	1.88	0.56
1:C:173:THR:HG22	1:C:182:MET:CE	2.36	0.55
1:C:44:PRO:HA	1:C:82:VAL:HG22	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:PRO:C	1:C:160:ASN:HD22	2.14	0.54
1:A:33:TYR:HB2	1:A:113:MET:HE2	1.90	0.54
1:A:282:GLN:HE21	1:A:282:GLN:N	2.00	0.54
1:B:227:ARG:HG3	1:B:227:ARG:NH1	2.22	0.54
1:C:280:GLN:CB	1:C:283:LEU:HD12	2.38	0.54
1:C:282:GLN:NE2	1:C:282:GLN:H	2.06	0.53
1:B:274:MET:HE2	1:B:285:GLN:HG3	1.90	0.53
1:C:43:THR:O	1:C:44:PRO:C	2.52	0.52
1:B:303:MET:HA	1:B:303:MET:CE	2.40	0.52
1:A:280:GLN:HB3	1:A:283:LEU:HD12	1.91	0.52
1:B:97:VAL:HA	1:B:215:ASN:HD21	1.74	0.52
1:C:282:GLN:H	1:C:282:GLN:HE21	1.57	0.52
1:B:215:ASN:N	1:B:215:ASN:HD22	2.09	0.51
1:B:303:MET:HE3	1:B:303:MET:HA	1.93	0.51
1:C:227:ARG:HG3	1:C:227:ARG:NH1	2.25	0.51
1:C:78:ILE:HD12	1:C:83:ARG:NE	2.26	0.51
1:B:104:TYR:CG	1:B:105:PRO:HD2	2.45	0.51
1:C:212:ASN:OD1	1:C:212:ASN:O	2.28	0.51
1:A:227:ARG:CB	1:A:227:ARG:NH1	2.69	0.51
1:C:285:GLN:O	1:C:286:PRO:C	2.52	0.50
1:A:274:MET:HE3	1:A:288:LYS:HB3	1.92	0.50
1:A:55:HIS:HD2	1:A:56:ASP:O	1.93	0.50
1:A:301:GLY:HA2	1:B:303:MET:HB2	1.92	0.50
1:A:303:MET:HA	1:A:303:MET:CE	2.41	0.50
1:B:33:TYR:HB2	1:B:113:MET:HE2	1.94	0.50
1:A:26:THR:C	1:A:27:HIS:HD2	2.20	0.50
1:A:194:SER:O	1:A:195:GLY:C	2.55	0.50
1:B:227:ARG:HH11	1:B:227:ARG:HB2	1.77	0.50
1:C:98:PHE:H	1:C:215:ASN:HD21	1.59	0.50
1:C:31:THR:OG1	1:C:34:GLY:O	2.28	0.49
1:C:120:TYR:C	1:C:120:TYR:CD1	2.90	0.49
1:C:265:ASP:OD1	1:C:267:THR:OG1	2.30	0.49
1:B:52:LEU:C	1:B:52:LEU:HD23	2.37	0.49
1:B:280:GLN:CB	1:B:283:LEU:HD12	2.42	0.49
1:B:53:THR:HA	1:B:129:VAL:O	2.12	0.48
1:C:231:PHE:O	1:C:263:LYS:HD3	2.13	0.48
1:A:52:LEU:C	1:A:52:LEU:HD23	2.38	0.48
1:C:52:LEU:C	1:C:52:LEU:HD23	2.39	0.48
1:C:33:TYR:HB2	1:C:113:MET:HE2	1.96	0.48
1:B:227:ARG:HH11	1:B:227:ARG:CG	2.28	0.47
1:B:280:GLN:NE2	1:B:282:GLN:NE2	2.55	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:ARG:HH11	1:C:227:ARG:CG	2.27	0.47
1:A:107:LEU:HD11	1:A:223:TYR:HA	1.96	0.47
1:C:45:LYS:HE3	1:C:80:ASN:HA	1.96	0.47
1:A:107:LEU:HD12	1:A:226:ARG:HB3	1.95	0.47
1:A:25:LYS:HB3	1:A:27:HIS:HE2	1.80	0.47
1:A:121:LEU:O	1:A:122:ASN:HB2	2.15	0.47
1:A:120:TYR:CD2	1:A:120:TYR:C	2.93	0.46
1:C:215:ASN:HD22	1:C:215:ASN:N	2.13	0.46
1:A:26:THR:C	1:A:27:HIS:CD2	2.94	0.46
1:B:232:GLU:OE1	1:B:235:GLY:HA3	2.15	0.46
1:B:194:SER:O	1:B:195:GLY:C	2.59	0.46
1:A:282:GLN:NE2	1:A:282:GLN:N	2.62	0.46
1:C:26:THR:O	1:C:27:HIS:CD2	2.64	0.46
1:C:227:ARG:NH1	1:C:227:ARG:CG	2.78	0.45
1:B:226:ARG:HG2	1:B:226:ARG:NH1	2.32	0.45
1:B:140:ARG:NH2	1:B:229:LEU:HD23	2.32	0.45
1:C:293:PHE:O	1:C:297:LEU:HG	2.17	0.45
1:C:107:LEU:HD11	1:C:223:TYR:HA	1.98	0.45
1:A:154:LEU:HD13	1:A:157:ILE:HD13	1.98	0.45
1:B:227:ARG:NH1	1:B:227:ARG:CG	2.79	0.44
1:C:118:LEU:HD23	1:C:118:LEU:HA	1.80	0.44
1:C:242:PRO:HA	1:C:268:GLN:O	2.17	0.44
1:A:114:ILE:O	1:A:115:PRO:C	2.60	0.44
1:A:140:ARG:NH2	1:A:229:LEU:HD23	2.33	0.44
1:A:284:THR:O	1:A:285:GLN:HG3	2.17	0.44
1:A:159:PRO:C	1:A:160:ASN:HD22	2.26	0.44
1:C:210:ALA:C	1:C:212:ASN:H	2.24	0.44
1:A:221:ASN:HB2	3:A:2023:HOH:O	2.17	0.44
1:C:78:ILE:C	1:C:80:ASN:H	2.26	0.44
1:A:45:LYS:HG3	1:A:80:ASN:O	2.18	0.43
1:B:121:LEU:O	1:B:122:ASN:HB2	2.17	0.43
1:C:45:LYS:HA	1:C:46:PRO:HD3	1.82	0.43
1:C:133:ALA:O	1:C:137:ILE:HG13	2.19	0.43
1:B:274:MET:HE3	1:B:288:LYS:HB3	1.99	0.43
1:C:160:ASN:HD22	1:C:160:ASN:N	2.15	0.43
1:A:250:GLN:NE2	3:A:2031:HOH:O	2.31	0.43
1:A:58:GLY:HA2	1:A:216:ILE:HD13	2.01	0.43
1:A:118:LEU:HD23	1:A:118:LEU:HA	1.80	0.43
1:C:114:ILE:O	1:C:115:PRO:C	2.60	0.43
1:A:97:VAL:HA	1:A:215:ASN:HD21	1.83	0.42
1:A:181:GLU:CG	3:A:2013:HOH:O	2.67	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:PHE:CE2	1:A:287:GLY:HA2	2.54	0.42
1:B:158:ASP:CG	1:B:226:ARG:HH21	2.27	0.42
1:A:202:LYS:O	1:A:205:ASN:HB3	2.20	0.42
1:B:181:GLU:HG2	3:B:2011:HOH:O	2.18	0.42
1:A:280:GLN:CB	1:A:283:LEU:HD12	2.49	0.42
1:A:301:GLY:O	1:B:48:ARG:NH2	2.52	0.42
1:B:78:ILE:C	1:B:80:ASN:N	2.76	0.42
1:A:60:ASN:O	1:A:61:TYR:C	2.63	0.42
1:B:229:LEU:HD13	1:B:231:PHE:CZ	2.55	0.42
1:C:232:GLU:OE1	1:C:235:GLY:HA3	2.20	0.42
1:A:303:MET:HB2	1:B:301:GLY:HA2	2.01	0.42
1:A:44:PRO:HA	1:A:82:VAL:HG22	2.00	0.42
1:A:285:GLN:O	1:A:286:PRO:C	2.63	0.42
1:B:107:LEU:HD12	1:B:226:ARG:HB3	2.01	0.41
1:B:250:GLN:NE2	3:B:2018:HOH:O	2.49	0.41
1:A:44:PRO:O	1:A:45:LYS:HD3	2.20	0.41
1:A:265:ASP:OD1	1:A:267:THR:OG1	2.30	0.41
1:C:194:SER:O	1:C:195:GLY:C	2.63	0.41
1:A:104:TYR:CG	1:A:105:PRO:HD2	2.56	0.41
1:A:251:ALA:HB1	1:A:252:PRO:CD	2.50	0.41
1:B:118:LEU:HA	1:B:118:LEU:HD23	1.78	0.41
1:B:132:GLY:C	1:B:134:GLY:N	2.79	0.41
1:C:227:ARG:HH11	1:C:227:ARG:CB	2.32	0.41
1:C:280:GLN:O	1:C:283:LEU:N	2.46	0.41
1:B:242:PRO:HA	1:B:268:GLN:O	2.21	0.41
1:B:282:GLN:OE1	1:B:282:GLN:N	2.52	0.41
1:C:221:ASN:O	1:C:222:SER:C	2.64	0.41
1:A:31:THR:HB	1:A:32:PRO:HD2	2.03	0.40
1:B:194:SER:C	1:B:196:ASN:N	2.78	0.40
1:C:66:GLN:O	1:C:67:PRO:C	2.61	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	279/281 (99%)	267 (96%)	12 (4%)	0	100	100
1	B	279/281 (99%)	265 (95%)	13 (5%)	1 (0%)	30	58
1	C	279/281 (99%)	262 (94%)	16 (6%)	1 (0%)	30	58
All	All	837/843 (99%)	794 (95%)	41 (5%)	2 (0%)	43	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	79	GLN
1	B	197	SER

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	240/240 (100%)	213 (89%)	27 (11%)	5	18
1	B	240/240 (100%)	212 (88%)	28 (12%)	5	17
1	C	240/240 (100%)	212 (88%)	28 (12%)	5	17
All	All	720/720 (100%)	637 (88%)	83 (12%)	5	17

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LYS
1	A	37	THR
1	A	43	THR
1	A	47	LYS
1	A	48	ARG
1	A	62	LYS
1	A	72	GLU
1	A	76	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	79	GLN
1	A	80	ASN
1	A	82	VAL
1	A	100	LEU
1	A	147	ASP
1	A	172	LEU
1	A	176	THR
1	A	190	GLN
1	A	194	SER
1	A	198	GLU
1	A	222	SER
1	A	227	ARG
1	A	238	THR
1	A	259	GLU
1	A	263	LYS
1	A	273	LYS
1	A	282	GLN
1	A	288	LYS
1	A	303	MET
1	B	25	LYS
1	B	37	THR
1	B	43	THR
1	B	47	LYS
1	B	48	ARG
1	B	62	LYS
1	B	72	GLU
1	B	76	GLU
1	B	79	GLN
1	B	82	VAL
1	B	100	LEU
1	B	103	GLN
1	B	120	TYR
1	B	147	ASP
1	B	156	ASN
1	B	172	LEU
1	B	176	THR
1	B	177	SER
1	B	181	GLU
1	B	190	GLN
1	B	194	SER
1	B	198	GLU
1	B	215	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	227	ARG
1	B	259	GLU
1	B	263	LYS
1	B	288	LYS
1	B	303	MET
1	C	25	LYS
1	C	30	GLU
1	C	43	THR
1	C	47	LYS
1	C	48	ARG
1	C	62	LYS
1	C	72	GLU
1	C	76	GLU
1	C	79	GLN
1	C	80	ASN
1	C	82	VAL
1	C	100	LEU
1	C	120	TYR
1	C	147	ASP
1	C	172	LEU
1	C	176	THR
1	C	182	MET
1	C	190	GLN
1	C	194	SER
1	C	198	GLU
1	C	215	ASN
1	C	227	ARG
1	C	240	ARG
1	C	259	GLU
1	C	273	LYS
1	C	282	GLN
1	C	288	LYS
1	C	300	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	HIS
1	A	75	GLN
1	A	79	GLN
1	A	144	ASN
1	A	160	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	201	GLN
1	A	209	HIS
1	A	250	GLN
1	A	280	GLN
1	A	282	GLN
1	A	298	GLN
1	B	79	GLN
1	B	156	ASN
1	B	160	ASN
1	B	215	ASN
1	B	224	ASN
1	B	280	GLN
1	B	298	GLN
1	C	27	HIS
1	C	75	GLN
1	C	79	GLN
1	C	156	ASN
1	C	160	ASN
1	C	170	HIS
1	C	201	GLN
1	C	215	ASN
1	C	218	ASN
1	C	221	ASN
1	C	253	HIS
1	C	280	GLN
1	C	282	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 [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	ACT	A	1305	-	3,3,3	0.56	0	3,3,3	1.80	1 (33%)
2	ACT	C	1305	-	3,3,3	1.39	1 (33%)	3,3,3	0.99	0
2	ACT	B	1305	-	3,3,3	0.94	0	3,3,3	0.33	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1305	ACT	O-C	2.26	1.32	1.22

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1305	ACT	OXT-C-CH3	2.51	125.59	115.05

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 [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	281/281 (100%)	-0.38	2 (0%) 84 78	24, 40, 59, 76	0
1	B	281/281 (100%)	-0.29	3 (1%) 78 70	23, 41, 59, 76	1 (0%)
1	C	281/281 (100%)	-0.32	3 (1%) 78 70	23, 41, 59, 76	1 (0%)
All	All	843/843 (100%)	-0.33	8 (0%) 81 74	23, 41, 59, 76	2 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	304	ALA	3.5
1	C	303	MET	3.1
1	C	44	PRO	2.7
1	B	44	PRO	2.3
1	B	24	ALA	2.3
1	A	30	GLU	2.2
1	B	46	PRO	2.2
1	A	44	PRO	2.1

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
2	ACT	C	1305	4/4	0.89	0.09	30,33,34,34	0
2	ACT	B	1305	4/4	0.96	0.07	30,31,31,31	0
2	ACT	A	1305	4/4	0.97	0.07	46,46,47,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.