



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 09:17 AM GMT

PDB ID : 2XMQ  
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 validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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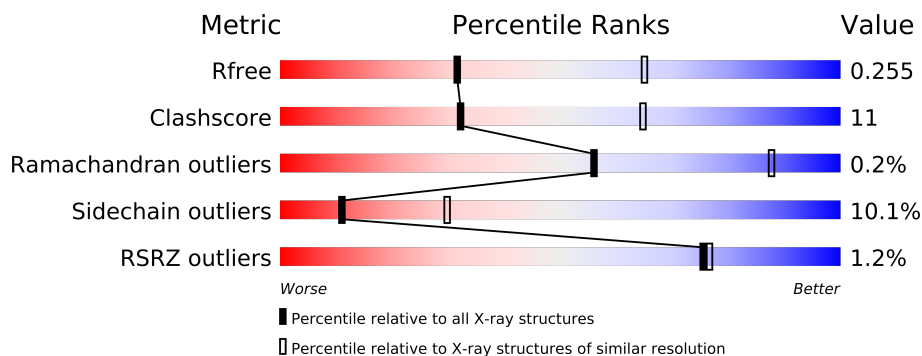
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1963 (2.84-2.80)
Clashscore	79885	2478 (2.84-2.80)
Ramachandran outliers	78287	2429 (2.84-2.80)
Sidechain outliers	78261	2431 (2.84-2.80)
RSRZ outliers	66119	1966 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	281	
1	B	281	
1	C	281	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 6720 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

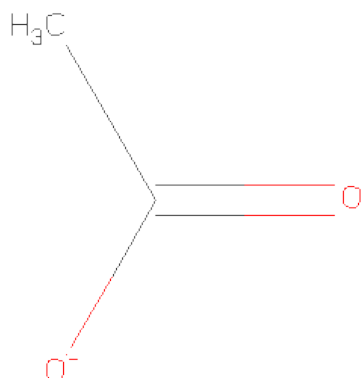
- Molecule 1 is a protein called PROTEIN NDRG2.

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 (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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.

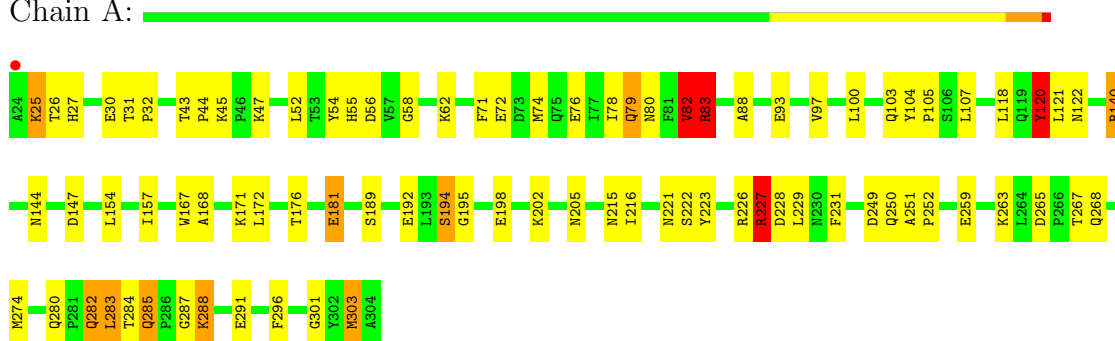
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	36	Total O 36 36	0	0
3	B	23	Total O 23 23	0	0
3	C	34	Total O 34 34	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

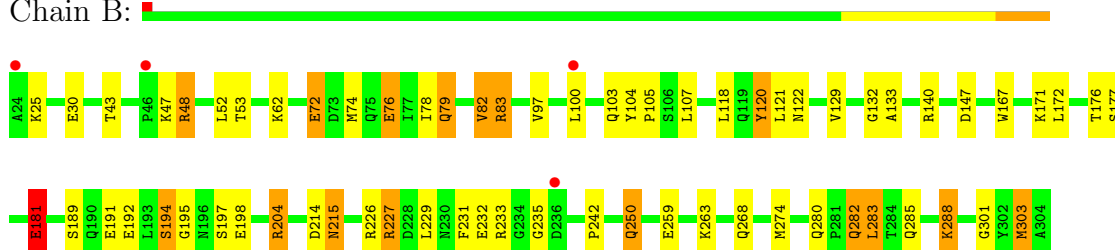
#### • Molecule 1: PROTEIN NDRG2

Chain A:



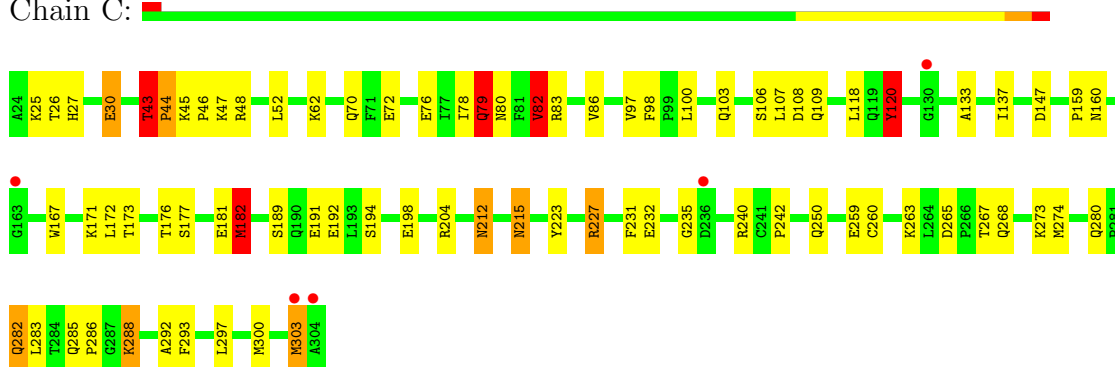
#### • Molecule 1: PROTEIN NDRG2

Chain B:



#### • Molecule 1: PROTEIN NDRG2

Chain C:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.41Å 88.90Å 126.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.81 29.86 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.2 (40.00-2.81) 99.2 (29.86-2.81)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.93 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.201 , 0.258 0.202 , 0.255	Depositor DCC
$R_{free}$ test set	1242 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.9	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 8.7	EDS
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 24312 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6720	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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: 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	1.39	18/2263 (0.8%)	1.17	15/3080 (0.5%)
1	B	1.33	10/2263 (0.4%)	1.12	10/3080 (0.3%)
1	C	1.37	14/2263 (0.6%)	1.17	11/3080 (0.4%)
All	All	1.36	42/6789 (0.6%)	1.16	36/9240 (0.4%)

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 (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	120	TYR	CE2-CZ	-9.97	1.25	1.38
1	A	120	TYR	CE1-CZ	-9.88	1.25	1.38
1	A	103	GLN	CB-CG	-8.76	1.28	1.52
1	A	30	GLU	CD-OE2	8.53	1.35	1.25
1	A	120	TYR	CG-CD1	-8.37	1.28	1.39
1	C	204	ARG	CZ-NH1	-8.19	1.22	1.33
1	A	120	TYR	CG-CD2	-8.17	1.28	1.39
1	B	191	GLU	CG-CD	8.15	1.64	1.51
1	B	181	GLU	CD-OE2	-7.55	1.17	1.25
1	A	30	GLU	CD-OE1	7.53	1.33	1.25
1	C	212	ASN	CB-CG	-7.39	1.34	1.51
1	C	212	ASN	CG-OD1	-7.18	1.08	1.24
1	B	120	TYR	CE2-CZ	-6.83	1.29	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	181	GLU	CB-CG	6.80	1.65	1.52
1	B	30	GLU	CG-CD	-6.73	1.41	1.51
1	C	260	CYS	CB-SG	-6.58	1.71	1.82
1	B	120	TYR	CG-CD1	-6.57	1.30	1.39
1	B	120	TYR	CG-CD2	-6.55	1.30	1.39
1	C	250	GLN	CG-CD	6.38	1.65	1.51
1	B	76	GLU	CG-CD	6.32	1.61	1.51
1	A	168	ALA	CA-CB	-6.29	1.39	1.52
1	C	62	LYS	CD-CE	6.05	1.66	1.51
1	A	268	GLN	CD-OE1	-6.04	1.10	1.24
1	B	72	GLU	CD-OE1	5.84	1.32	1.25
1	C	181	GLU	CG-CD	5.77	1.60	1.51
1	A	93	GLU	CD-OE2	5.75	1.31	1.25
1	C	250	GLN	CB-CG	5.75	1.68	1.52
1	C	191	GLU	CG-CD	5.50	1.60	1.51
1	C	30	GLU	CG-CD	-5.49	1.43	1.51
1	A	144	ASN	CG-ND2	-5.47	1.19	1.32
1	A	296	PHE	CE1-CZ	5.44	1.47	1.37
1	C	292	ALA	CA-CB	-5.42	1.41	1.52
1	A	291	GLU	CD-OE2	5.40	1.31	1.25
1	C	70	GLN	CD-OE1	-5.38	1.12	1.24
1	A	25	LYS	CD-CE	5.37	1.64	1.51
1	A	54	TYR	CG-CD2	5.37	1.46	1.39
1	B	250	GLN	CB-CG	5.36	1.67	1.52
1	C	86	VAL	CB-CG1	-5.36	1.41	1.52
1	C	120	TYR	CG-CD1	-5.32	1.32	1.39
1	A	285	GLN	CG-CD	-5.25	1.39	1.51
1	B	282	GLN	CD-OE1	-5.16	1.12	1.24
1	A	285	GLN	CD-OE1	-5.05	1.12	1.24

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	204	ARG	NE-CZ-NH2	13.78	127.19	120.30
1	B	204	ARG	NE-CZ-NH2	10.10	125.35	120.30
1	C	182	MET	CB-CG-SD	8.28	137.24	112.40
1	A	285	GLN	CA-CB-CG	-8.14	95.50	113.40
1	A	103	GLN	N-CA-CB	-8.10	96.03	110.60
1	C	212	ASN	N-CA-CB	-8.07	96.07	110.60
1	A	227	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	C	182	MET	CG-SD-CE	-7.77	87.76	100.20
1	B	30	GLU	CA-CB-CG	-7.48	96.94	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	181	GLU	OE1-CD-OE2	-7.38	114.44	123.30
1	B	181	GLU	CG-CD-OE1	6.97	132.24	118.30
1	A	140	ARG	NE-CZ-NH2	-6.93	116.84	120.30
1	C	181	GLU	OE1-CD-OE2	-6.77	115.18	123.30
1	C	212	ASN	CB-CG-OD1	-6.75	108.11	121.60
1	B	204	ARG	NE-CZ-NH1	-6.60	117.00	120.30
1	A	30	GLU	CA-CB-CG	-6.52	99.06	113.40
1	C	30	GLU	CA-CB-CG	-6.42	99.26	113.40
1	A	82	VAL	CB-CA-C	-6.18	99.65	111.40
1	A	30	GLU	OE1-CD-OE2	6.14	130.66	123.30
1	C	108	ASP	CB-CG-OD2	5.94	123.65	118.30
1	C	43	THR	N-CA-C	-5.78	95.39	111.00
1	A	227	ARG	CG-CD-NE	5.77	123.92	111.80
1	A	227	ARG	CD-NE-CZ	5.70	131.58	123.60
1	B	214	ASP	CB-CG-OD1	-5.69	113.18	118.30
1	B	214	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	181	GLU	OE1-CD-OE2	-5.58	116.60	123.30
1	A	83	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	283	LEU	CB-CG-CD1	-5.32	101.96	111.00
1	B	82	VAL	CB-CA-C	-5.30	101.33	111.40
1	A	283	LEU	CB-CG-CD1	-5.27	102.05	111.00
1	B	30	GLU	OE1-CD-OE2	5.26	129.61	123.30
1	A	181	GLU	CG-CD-OE1	5.12	128.53	118.30
1	A	228	ASP	CB-CG-OD2	5.11	122.89	118.30
1	C	303	MET	CG-SD-CE	5.11	108.37	100.20
1	A	249	ASP	CB-CG-OD1	5.10	122.89	118.30
1	C	82	VAL	CB-CA-C	-5.05	101.81	111.40

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2205	0	2142	58	0
1	B	2205	0	2142	45	0
1	C	2205	0	2142	52	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	149	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (149) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:79:GLN:HA	1:B:79:GLN:NE2	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:HE21	1:A:79:GLN:HA	1.32	0.94
1:A:227:ARG:HH11	1:A:227:ARG:HB3	1.34	0.91
1:C:79:GLN:HA	1:C:79:GLN:NE2	1.85	0.89
1:A:282:GLN:H	1:A:282:GLN:HE21	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:B:280:GLN:NE2	1:B:282:GLN:HE22	1.78	0.81
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:B:303:MET:HE3	1:B:303:MET:HA	1.68	0.76
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:A:303:MET:HA	1:A:303:MET:HE3	1.71	0.71
1:B:181:GLU:OE1	1:B:204:ARG:NH1	2.26	0.69
1:A:282:GLN:NE2	1:A:282:GLN:H	1.91	0.69
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:303:MET:CE	1:C:303:MET:HA	2.26	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:A:27:HIS:HD1	1:A:120:TYR:HH	1.45	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:A:231:PHE:O	1:A:263:LYS:HD3	2.01	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:B:274:MET:HE2	1:B:285:GLN:HG3	1.84	0.58
1:C:167:TRP:O	1:C:171:LYS:CG	2.46	0.57
1:C:227:ARG:HH11	1:C:227:ARG:HB2	1.69	0.57
1:C:280:GLN:HB3	1:C:283:LEU:HD12	1.86	0.57
1:A:189:SER:OG	1:A:192:GLU:HG3	2.05	0.57
1:A:74:MET:O	1:A:78:ILE:HG12	2.04	0.57
1:C:173:THR:HG22	1:C:182:MET:CE	2.36	0.56
1:B:83:ARG:HD3	1:B:83:ARG:N	2.21	0.56
1:B:226:ARG:HH11	1:B:226:ARG:HG2	1.70	0.56
1:A:83:ARG:HD3	1:A:83:ARG:N	2.21	0.56
1:C:177:SER:HB2	1:C:182:MET:HE1	1.86	0.56
1:C:44:PRO:HA	1:C:82:VAL:HG22	1.89	0.54
1:A:282:GLN:N	1:A:282:GLN:HE21	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:H	1:C:282:GLN:NE2	2.06	0.53
1:A:284:THR:C	1:A:285:GLN:HG3	2.28	0.53
1:C:212:ASN:C	1:C:212:ASN:OD1	2.43	0.53
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:132:GLY:O	1:B:133:ALA:C	2.46	0.51
1:B:215:ASN:HD22	1:B:215:ASN:N	2.09	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:C:212:ASN:O	1:C:212:ASN:OD1	2.28	0.51
1:B:104:TYR:CG	1:B:105:PRO:HD2	2.45	0.51
1:A:227:ARG:CB	1:A:227:ARG:NH1	2.69	0.51
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:CE	1:A:303:MET:HA	2.41	0.50
1:C:274:MET:HE3	1:C:288:LYS:HB3	1.92	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:98:PHE:H	1:C:215:ASN:HD21	1.59	0.50
1:B:227:ARG:HH11	1:B:227:ARG:HB2	1.77	0.50
1:B:303:MET:CE	1:B:303:MET:HA	2.40	0.49
1:C:159:PRO:C	1:C:160:ASN:HD22	2.14	0.49
1:B:280:GLN:CB	1:B:283:LEU:HD12	2.42	0.49
1:A:303:MET:SD	1:B:303:MET:HE3	2.53	0.48
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:27:HIS:ND1	1:A:120:TYR:OH	2.46	0.48
1:A:274:MET:HE3	1:A:288:LYS:HB3	1.95	0.48
1:C:43:THR:O	1:C:44:PRO:C	2.52	0.48
1:B:280:GLN:NE2	1:B:282:GLN:NE2	2.55	0.47
1:B:227:ARG:HH11	1:B:227:ARG:CG	2.28	0.47
1:C:227:ARG:HH11	1:C:227:ARG:CG	2.27	0.47
1:C:173:THR:CG2	1:C:182:MET:HE2	2.45	0.47
1:C:45:LYS:HE3	1:C:80:ASN:HA	1.96	0.47
1:A:107:LEU:HD11	1:A:223:TYR:HA	1.96	0.47
1:A:107:LEU:HD12	1:A:226:ARG:HB3	1.95	0.47
1:A:121:LEU:O	1:A:122:ASN:HB2	2.15	0.47
1:C:215:ASN:N	1:C:215:ASN:HD22	2.13	0.46
1:C:285:GLN:O	1:C:286:PRO:C	2.52	0.46
1:C:177:SER:HB2	1:C:182:MET:HE3	1.98	0.46
1:A:303:MET:HE3	1:B:303:MET:SD	2.56	0.46
1:B:232:GLU:OE1	1:B:235:GLY:HA3	2.15	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:173:THR:HG22	1:C:182:MET:HE2	1.97	0.46
1:C:227:ARG:CG	1:C:227:ARG:NH1	2.78	0.45
1:A:26:THR:C	1:A:27:HIS:HD2	2.20	0.45
1:C:173:THR:HG22	1:C:182:MET:HE1	1.99	0.45
1:B:226:ARG:HG2	1:B:226:ARG:NH1	2.32	0.45
1:A:194:SER:O	1:A:195:GLY:C	2.55	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:B:274:MET:HE3	1:B:288:LYS:HD2	1.98	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:C:120:TYR:C	1:C:120:TYR:CD1	2.90	0.45
1:C:177:SER:CB	1:C:182:MET:HE3	2.47	0.44
1:B:52:LEU:HD23	1:B:52:LEU:C	2.37	0.44
1:B:227:ARG:CG	1:B:227:ARG:NH1	2.79	0.44
1:C:242:PRO:HA	1:C:268:GLN:O	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:118:LEU:HD23	1:C:118:LEU:HA	1.80	0.44
1:A:284:THR:O	1:A:285:GLN:HG3	2.17	0.44
1:A:140:ARG:NH2	1:A:229:LEU:HD23	2.33	0.44
1:A:221:ASN:HB2	3:A:2023:HOH:O	2.17	0.44
1:A:45:LYS:HG3	1:A:80:ASN:O	2.18	0.43
1:C:45:LYS:HA	1:C:46:PRO:HD3	1.82	0.43
1:B:121:LEU:O	1:B:122:ASN:HB2	2.17	0.43
1:C:133:ALA:O	1:C:137:ILE:HG13	2.19	0.43
1:C:52:LEU:HD23	1:C:52:LEU:C	2.39	0.43
1:A:52:LEU:C	1:A:52:LEU:HD23	2.38	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:118:LEU:HA	1:A:118:LEU:HD23	1.80	0.43
1:A:58:GLY:HA2	1:A:216:ILE:HD13	2.01	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
1:A:71:PHE:CE2	1:A:287:GLY:HA2	2.54	0.42
1:B:181:GLU:HG2	3:B:2011:HOH:O	2.18	0.42
1:A:202:LYS:O	1:A:205:ASN:HB3	2.20	0.42
1:A:301:GLY:O	1:B:48:ARG:NH2	2.52	0.42
1:A:280:GLN:CB	1:A:283:LEU:HD12	2.49	0.42
1:C:265:ASP:OD1	1:C:267:THR:OG1	2.30	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:120:TYR:CD2	1:A:120:TYR:C	2.93	0.42
1:A:44:PRO:HA	1:A:82:VAL:HG22	2.00	0.42
1:B:107:LEU:HD12	1:B:226:ARG:HB3	2.01	0.41
1:A:26:THR:C	1:A:27:HIS:CD2	2.94	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:A:104:TYR:CG	1:A:105:PRO:HD2	2.56	0.41
1:B:194:SER:O	1:B:195:GLY:C	2.59	0.41
1:A:251:ALA:HB1	1:A:252:PRO:CD	2.50	0.41
1:A:27:HIS:HD1	1:A:120:TYR:HE2	1.68	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:118:LEU:HA	1:B:118:LEU:HD23	1.78	0.41
1:B:282:GLN:N	1:B:282:GLN:OE1	2.52	0.41
1:B:242:PRO:HA	1:B:268:GLN:O	2.21	0.41
1:A:31:THR:HB	1:A:32:PRO:HD2	2.03	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%)	43	79
1	C	279/281 (99%)	262 (94%)	16 (6%)	1 (0%)	43	79
All	All	837/843 (99%)	794 (95%)	41 (5%)	2 (0%)	56	88

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%)	218 (91%)	22 (9%)	13	36
1	B	240/240 (100%)	215 (90%)	25 (10%)	10	28
1	C	240/240 (100%)	214 (89%)	26 (11%)	9	26
All	All	720/720 (100%)	647 (90%)	73 (10%)	11	30

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LYS

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Mol	Chain	Res	Type
1	A	43	THR
1	A	47	LYS
1	A	62	LYS
1	A	72	GLU
1	A	76	GLU
1	A	79	GLN
1	A	82	VAL
1	A	83	ARG
1	A	100	LEU
1	A	120	TYR
1	A	147	ASP
1	A	172	LEU
1	A	176	THR
1	A	194	SER
1	A	198	GLU
1	A	222	SER
1	A	227	ARG
1	A	259	GLU
1	A	282	GLN
1	A	288	LYS
1	A	303	MET
1	B	25	LYS
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	83	ARG
1	B	100	LEU
1	B	103	GLN
1	B	120	TYR
1	B	147	ASP
1	B	172	LEU
1	B	176	THR
1	B	177	SER
1	B	181	GLU
1	B	194	SER
1	B	198	GLU
1	B	215	ASN

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Mol	Chain	Res	Type
1	B	227	ARG
1	B	259	GLU
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	72	GLU
1	C	76	GLU
1	C	79	GLN
1	C	82	VAL
1	C	100	LEU
1	C	103	GLN
1	C	120	TYR
1	C	147	ASP
1	C	172	LEU
1	C	176	THR
1	C	182	MET
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	HIS
1	A	79	GLN
1	A	160	ASN
1	A	190	GLN
1	A	201	GLN
1	A	209	HIS
1	A	280	GLN
1	A	282	GLN

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Mol	Chain	Res	Type
1	A	298	GLN
1	B	27	HIS
1	B	79	GLN
1	B	156	ASN
1	B	160	ASN
1	B	190	GLN
1	B	201	GLN
1	B	215	ASN
1	B	280	GLN
1	B	298	GLN
1	C	27	HIS
1	C	70	GLN
1	C	79	GLN
1	C	160	ASN
1	C	201	GLN
1	C	215	ASN
1	C	221	ASN
1	C	280	GLN
1	C	282	GLN
1	C	298	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	-	1,3,3	1.24	0	0,3,3	0.00	-
2	ACT	B	1305	-	1,3,3	0.36	0	0,3,3	0.00	-
2	ACT	C	1305	-	1,3,3	2.17	1 (100%)	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACT	A	1305	-	-	0/0/0/0	0/0/0/0
2	ACT	B	1305	-	-	0/0/0/0	0/0/0/0
2	ACT	C	1305	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1305	ACT	CH3-C	2.17	1.51	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	281/281 (100%)	-0.31	1 (0%) 90 91	24, 40, 59, 76	0
1	B	281/281 (100%)	-0.24	4 (1%) 72 72	23, 41, 59, 76	1 (0%)
1	C	281/281 (100%)	-0.24	5 (1%) 65 66	23, 41, 59, 76	1 (0%)
All	All	843/843 (100%)	-0.26	10 (1%) 75 76	23, 41, 59, 76	2 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	304	ALA	4.6
1	B	24	ALA	3.2
1	B	100	LEU	3.2
1	B	236	ASP	2.8
1	C	236	ASP	2.8
1	C	130	GLY	2.5
1	C	303	MET	2.3
1	B	46	PRO	2.2
1	A	24	ALA	2.2
1	C	163	GLY	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ACT	A	1305	4/4	0.18	0.60	46,46,47,48	0
2	ACT	C	1305	4/4	0.12	-1.75	30,33,34,34	0
2	ACT	B	1305	4/4	0.10	-2.60	30,31,31,31	0

## 6.5 Other polymers

There are no such residues in this entry.