



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:53 AM GMT

PDB ID : 3NEZ  
Title : mRojoA  
Authors : Mayo, S.L.; Chica, R.A.; Moore, M.M.  
Deposited on : 2010-06-09  
Resolution : 1.70 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

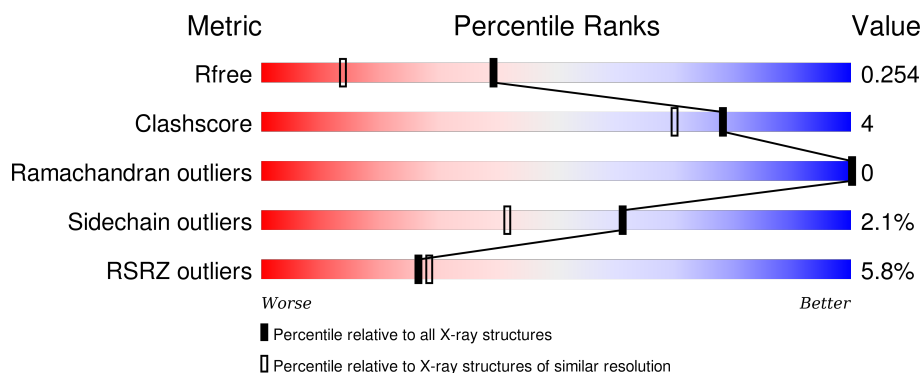
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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))
$R_{free}$	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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. 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	243	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>11%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	243	<div> <div>7%</div> <div> <div></div> <div>79%</div> <div>8%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	243	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>9%</div> <div>•</div> <div>11%</div> </div> </div>
1	D	243	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>11%</div> <div>•</div> <div>11%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7612 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 mRojoA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	35	9	0
			1802	1154	297	339	12			
1	B	215	Total	C	N	O	S	62	8	0
			1771	1139	287	335	10			
1	C	215	Total	C	N	O	S	72	4	0
			1763	1128	290	335	10			
1	D	216	Total	C	N	O	S	52	6	0
			1787	1141	299	337	10			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	NRQ	MET	CHROMOPHORE	PDB 3NEZ
A	67	NRQ	MET	MICROHETEROGENEITY	PDB 3NEZ
A	67	NRQ	TYR	CHROMOPHORE	PDB 3NEZ
A	67	NRQ	TYR	MICROHETEROGENEITY	PDB 3NEZ
A	67	NRQ	GLY	CHROMOPHORE	PDB 3NEZ
A	67	NRQ	GLY	MICROHETEROGENEITY	PDB 3NEZ
B	67	NRQ	MET	CHROMOPHORE	PDB 3NEZ
B	67	NRQ	MET	MICROHETEROGENEITY	PDB 3NEZ
B	67	NRQ	TYR	CHROMOPHORE	PDB 3NEZ
B	67	NRQ	TYR	MICROHETEROGENEITY	PDB 3NEZ
B	67	NRQ	GLY	CHROMOPHORE	PDB 3NEZ
B	67	NRQ	GLY	MICROHETEROGENEITY	PDB 3NEZ
C	67	NRQ	MET	CHROMOPHORE	PDB 3NEZ
C	67	NRQ	MET	MICROHETEROGENEITY	PDB 3NEZ
C	67	NRQ	TYR	CHROMOPHORE	PDB 3NEZ
C	67	NRQ	TYR	MICROHETEROGENEITY	PDB 3NEZ
C	67	NRQ	GLY	CHROMOPHORE	PDB 3NEZ
C	67	NRQ	GLY	MICROHETEROGENEITY	PDB 3NEZ
D	67	NRQ	MET	CHROMOPHORE	PDB 3NEZ
D	67	NRQ	MET	MICROHETEROGENEITY	PDB 3NEZ
D	67	NRQ	TYR	CHROMOPHORE	PDB 3NEZ

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Chain	Residue	Modelled	Actual	Comment	Reference
D	67	NRQ	TYR	MICROHETEROGENEITY	PDB 3NEZ
D	67	NRQ	GLY	CHROMOPHORE	PDB 3NEZ
D	67	NRQ	GLY	MICROHETEROGENEITY	PDB 3NEZ

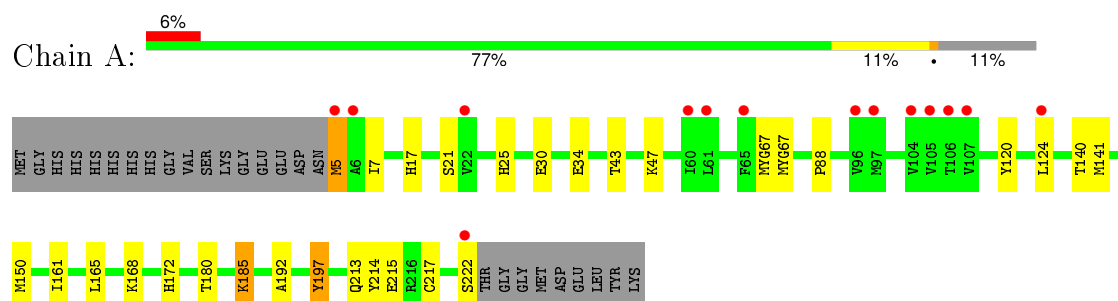
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	145	Total O 145 145	0	0
2	B	121	Total O 121 121	0	0
2	C	106	Total O 106 106	0	0
2	D	117	Total O 117 117	0	0

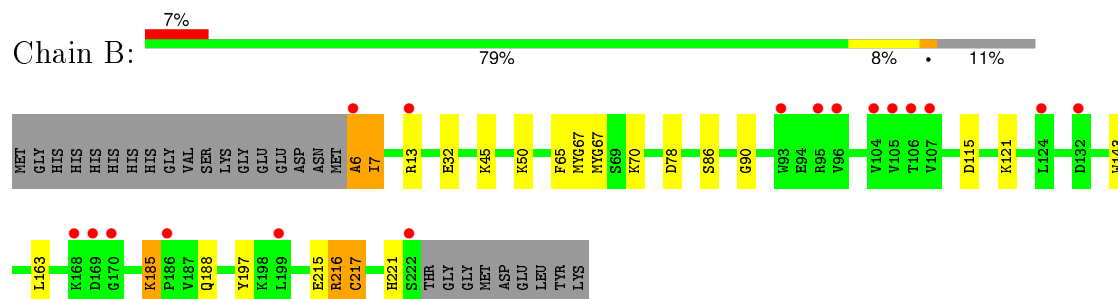
### 3 Residue-property plots [i](#)

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.

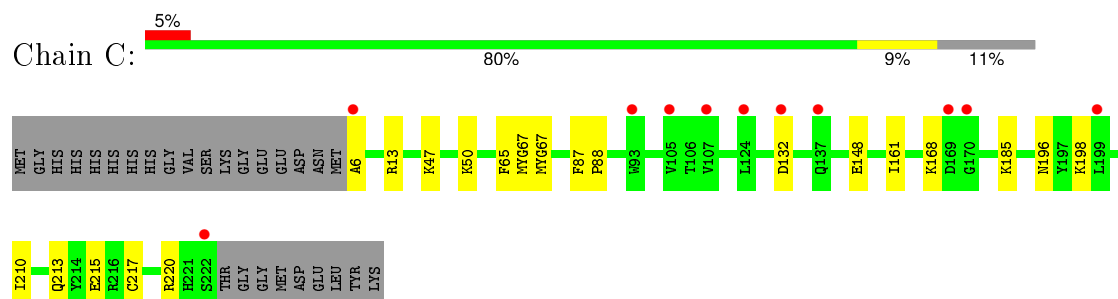
#### • Molecule 1: mRojoA



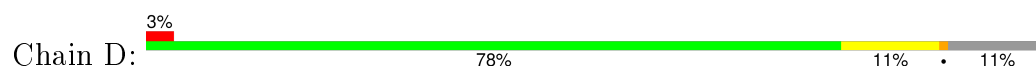
#### • Molecule 1: mRojoA

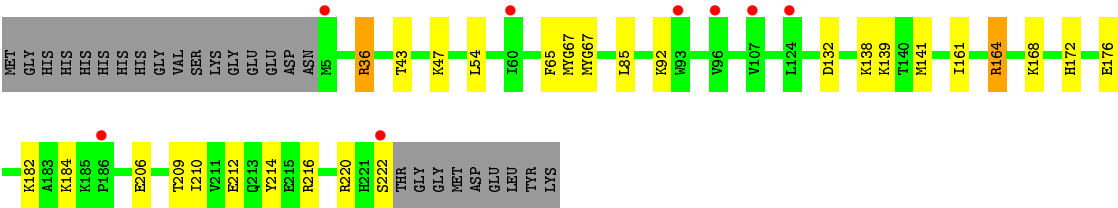


#### • Molecule 1: mRojoA



#### • Molecule 1: mRojoA





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.24Å 97.41Å 84.16Å 90.00° 95.54° 90.00°	Depositor
Resolution (Å)	30.48 – 1.70 30.48 – 1.70	Depositor EDS
% Data completeness (in resolution range)	95.2 (30.48-1.70) 95.2 (30.48-1.70)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, $R_{free}$	0.182 , 0.221 0.220 , 0.254	Depositor DCC
$R_{free}$ test set	5128 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.3	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 43.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 102731 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7612	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: NRQ, CH6

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	1.23	5/1827 (0.3%)	1.01	3/2458 (0.1%)
1	B	1.19	8/1795 (0.4%)	1.08	11/2417 (0.5%)
1	C	1.19	5/1775 (0.3%)	1.04	9/2388 (0.4%)
1	D	1.26	9/1810 (0.5%)	1.17	13/2434 (0.5%)
All	All	1.22	27/7207 (0.4%)	1.08	36/9697 (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

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	6	ALA	CA-CB	-17.14	1.16	1.52
1	B	188	GLN	CG-CD	14.84	1.85	1.51
1	D	222	SER	CB-OG	-12.84	1.25	1.42
1	D	176	GLU	CG-CD	12.51	1.70	1.51
1	D	182	LYS	CG-CD	-10.65	1.16	1.52
1	B	7	ILE	CB-CG1	-9.98	1.26	1.54
1	C	13	ARG	CZ-NH2	9.87	1.45	1.33
1	B	121	LYS	CD-CE	9.21	1.74	1.51
1	A	222	SER	CA-CB	8.19	1.65	1.52
1	C	50	LYS	CG-CD	8.07	1.79	1.52
1	D	47	LYS	CE-NZ	-8.06	1.28	1.49
1	C	198	LYS	CG-CD	7.67	1.78	1.52
1	B	185	LYS	CA-CB	-6.96	1.38	1.53
1	D	85	LEU	CG-CD1	6.64	1.76	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	120	TYR	CE1-CZ	6.63	1.47	1.38
1	B	45	LYS	CG-CD	6.60	1.74	1.52
1	A	7	ILE	CB-CG1	-6.50	1.35	1.54
1	D	139	LYS	CD-CE	6.48	1.67	1.51
1	B	6	ALA	CA-C	6.20	1.69	1.52
1	A	47	LYS	CD-CE	6.15	1.66	1.51
1	B	217[A]	CYS	CB-SG	5.86	1.92	1.82
1	B	217[B]	CYS	CB-SG	5.86	1.92	1.82
1	C	168	LYS	CE-NZ	-5.57	1.35	1.49
1	D	206	GLU	CB-CG	-5.56	1.41	1.52
1	A	34	GLU	CG-CD	-5.45	1.43	1.51
1	D	212	GLU	CG-CD	5.08	1.59	1.51
1	D	220	ARG	CG-CD	-5.03	1.39	1.51

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	132	ASP	CB-CG-OD2	-13.55	106.11	118.30
1	D	36	ARG	NE-CZ-NH2	12.81	126.70	120.30
1	B	6	ALA	CA-C-O	-10.53	98.00	120.10
1	D	220	ARG	CG-CD-NE	10.21	133.24	111.80
1	C	6	ALA	N-CA-CB	9.53	123.45	110.10
1	D	36	ARG	NE-CZ-NH1	-8.81	115.90	120.30
1	C	50	LYS	CB-CG-CD	-8.54	89.38	111.60
1	B	188	GLN	CB-CG-CD	-8.35	89.88	111.60
1	C	6	ALA	CB-CA-C	8.12	122.28	110.10
1	B	216	ARG	NE-CZ-NH2	-8.09	116.25	120.30
1	C	65[A]	PHE	CB-CG-CD2	-7.38	115.64	120.80
1	C	65[B]	PHE	CB-CG-CD2	-7.38	115.64	120.80
1	B	6	ALA	CB-CA-C	-7.13	99.40	110.10
1	C	198	LYS	CB-CG-CD	-7.12	93.10	111.60
1	C	65[A]	PHE	CB-CG-CD1	7.04	125.73	120.80
1	C	65[B]	PHE	CB-CG-CD1	7.04	125.73	120.80
1	B	7	ILE	CA-CB-CG2	-6.90	97.10	110.90
1	B	45	LYS	CB-CG-CD	-6.76	94.03	111.60
1	D	182	LYS	CB-CG-CD	6.74	129.13	111.60
1	B	216	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	D	85	LEU	CB-CG-CD1	-6.47	100.01	111.00
1	D	141	MET	CG-SD-CE	6.19	110.10	100.20
1	D	65[A]	PHE	CB-CG-CD2	-6.13	116.51	120.80
1	D	65[B]	PHE	CB-CG-CD2	-6.13	116.51	120.80
1	B	65[A]	PHE	CB-CG-CD1	5.84	124.89	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65[B]	PHE	CB-CG-CD1	5.84	124.89	120.80
1	D	164[A]	ARG	NE-CZ-NH2	5.78	123.19	120.30
1	D	164[B]	ARG	NE-CZ-NH2	5.78	123.19	120.30
1	A	222	SER	CB-CA-C	-5.54	99.58	110.10
1	A	222	SER	N-CA-CB	-5.38	102.42	110.50
1	B	188	GLN	CG-CD-OE1	-5.35	110.91	121.60
1	C	132	ASP	CB-CG-OD1	5.34	123.10	118.30
1	D	164[A]	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	D	164[B]	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	B	50	LYS	CD-CE-NZ	5.13	123.51	111.70
1	A	197	TYR	CB-CA-C	-5.06	100.29	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	6	ALA	Mainchain

## 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	1802	0	1746	21	2
1	B	1771	0	1710	6	0
1	C	1763	0	1692	9	0
1	D	1787	0	1721	8	2
2	A	145	0	0	6	0
2	B	121	0	0	0	0
2	C	106	0	0	0	1
2	D	117	0	0	2	1
All	All	7612	0	6869	44	3

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 4.

All (44) 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:C:47:LYS:HG2	1:C:210:ILE:HD13	1.45	0.99
1:D:36:ARG:HD2	2:D:425:HOH:O	1.72	0.89
1:A:5:MET:HA	1:A:88:PRO:HB2	1.65	0.77
1:A:5:MET:HA	1:A:88:PRO:CB	2.17	0.74
1:A:217[B]:CYS:SG	2:A:453:HOH:O	2.53	0.66
1:A:197:TYR:CD1	1:A:217[B]:CYS:SG	2.87	0.65
1:A:197:TYR:CE1	1:A:217[B]:CYS:SG	2.91	0.63
1:A:43[B]:THR:HG22	2:A:345:HOH:O	1.98	0.62
1:A:17:HIS:ND1	1:A:30:GLU:OE2	2.31	0.62
1:D:43[A]:THR:HG22	1:D:214:TYR:HD1	1.67	0.59
1:A:185:LYS:HD2	2:A:289:HOH:O	2.04	0.57
1:C:47:LYS:HG2	1:C:210:ILE:CD1	2.29	0.56
1:C:215:GLU:HG2	1:C:217[B]:CYS:SG	2.45	0.56
1:A:180[B]:THR:HG23	2:A:394:HOH:O	2.06	0.55
1:B:67[A]:NRQ:N1	1:B:67[A]:NRQ:CA3	2.69	0.55
1:D:138:LYS:NZ	1:D:138:LYS:HB3	2.22	0.55
1:D:54:LEU:HD12	2:D:428:HOH:O	2.05	0.54
1:C:67[A]:NRQ:N1	1:C:67[A]:NRQ:CA3	2.70	0.54
1:B:70:LYS:HD3	1:B:197:TYR:OH	2.08	0.53
1:A:43[A]:THR:HG22	1:A:214:TYR:HD1	1.73	0.53
1:B:78:ASP:OD1	1:B:221:HIS:NE2	2.42	0.53
1:B:86[B]:SER:OG	1:B:90:GLY:O	2.20	0.51
1:D:164[A]:ARG:HH12	1:D:172:HIS:CE1	2.28	0.51
1:B:215:GLU:HG2	1:B:217[B]:CYS:SG	2.52	0.50
1:C:67[A]:NRQ:N1	1:C:67[A]:NRQ:HA31	2.27	0.49
1:A:67[A]:NRQ:N1	1:A:67[A]:NRQ:C3	2.76	0.49
1:A:185:LYS:HE3	2:A:454:HOH:O	2.13	0.48
1:C:87:PHE:HB3	1:C:88:PRO:HA	1.97	0.47
1:D:92:LYS:HE2	1:D:184:LYS:HE2	1.97	0.47
1:A:141[A]:MET:HG3	1:A:168:LYS:HA	1.97	0.46
1:C:196:ASN:ND2	1:C:220:ARG:CD	2.78	0.46
1:A:150:MET:O	1:A:192:ALA:HA	2.16	0.45
1:A:43[A]:THR:HG23	2:A:345:HOH:O	2.17	0.44
1:A:215:GLU:HG2	1:A:217[B]:CYS:SG	2.57	0.44
1:A:140:THR:C	1:A:141[A]:MET:HG2	2.38	0.44
1:A:124:LEU:HD23	1:A:124:LEU:C	2.38	0.43
1:A:5:MET:HA	1:A:88:PRO:HB3	1.95	0.43
1:B:143:TRP:CZ3	1:B:163:LEU:HB3	2.54	0.43
1:D:209:THR:O	1:D:210:ILE:HD13	2.19	0.42
1:C:148:GLU:HG3	1:C:161:ILE:HG12	2.00	0.42
1:C:196:ASN:O	1:C:217[A]:CYS:HA	2.19	0.42
1:A:21:SER:HA	1:A:25:HIS:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:THR:HB	1:A:165:LEU:HG	2.02	0.41
1:D:67[A]:NRQ:N1	1:D:67[A]:NRQ:CA3	2.83	0.41

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172[B]:HIS:NE2	1:D:172:HIS:NE2[2_444]	1.72	0.48
1:A:172[B]:HIS:CD2	1:D:172:HIS:NE2[2_444]	1.99	0.21
2:C:413:HOH:O	2:D:425:HOH:O[1_455]	2.14	0.06

## 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	218/243 (90%)	213 (98%)	5 (2%)	0	100	100
1	B	216/243 (89%)	214 (99%)	2 (1%)	0	100	100
1	C	212/243 (87%)	209 (99%)	3 (1%)	0	100	100
1	D	215/243 (88%)	212 (99%)	3 (1%)	0	100	100
All	All	861/972 (89%)	848 (98%)	13 (2%)	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	191/204 (94%)	187 (98%)	4 (2%)	61	42
1	B	185/204 (91%)	179 (97%)	6 (3%)	46	24
1	C	184/204 (90%)	182 (99%)	2 (1%)	80	69
1	D	188/204 (92%)	185 (98%)	3 (2%)	70	54
All	All	748/816 (92%)	733 (98%)	15 (2%)	61	44

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	161	ILE
1	A	185	LYS
1	A	213	GLN
1	B	7	ILE
1	B	13	ARG
1	B	32	GLU
1	B	115	ASP
1	B	185	LYS
1	B	216	ARG
1	C	185	LYS
1	C	213	GLN
1	D	161	ILE
1	D	168	LYS
1	D	216	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	172	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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
1	CH6	A	67[B]	1	24,24,25	3.49	7 (29%)	28,32,34	3.70	11 (39%)
1	NRQ	A	67[A]	1	23,24,25	3.13	4 (17%)	23,32,34	3.59	10 (43%)
1	CH6	B	67[B]	1	24,24,25	3.24	7 (29%)	28,32,34	3.14	9 (32%)
1	NRQ	B	67[A]	1	23,24,25	3.14	6 (26%)	23,32,34	3.26	9 (39%)
1	CH6	C	67[B]	1	24,24,25	3.30	7 (29%)	28,32,34	4.16	11 (39%)
1	NRQ	C	67[A]	1	23,24,25	3.20	6 (26%)	23,32,34	4.44	11 (47%)
1	CH6	D	67[B]	1	24,24,25	3.78	6 (25%)	28,32,34	4.04	11 (39%)
1	NRQ	D	67[A]	1	23,24,25	3.48	4 (17%)	23,32,34	3.89	8 (34%)

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
1	CH6	A	67[B]	1	-	0/11/31/32	0/2/2/2
1	NRQ	A	67[A]	1	-	0/9/31/32	0/2/2/2
1	CH6	B	67[B]	1	-	0/11/31/32	0/2/2/2
1	NRQ	B	67[A]	1	-	0/9/31/32	0/2/2/2
1	CH6	C	67[B]	1	-	0/11/31/32	0/2/2/2
1	NRQ	C	67[A]	1	-	0/9/31/32	0/2/2/2
1	CH6	D	67[B]	1	-	0/11/31/32	0/2/2/2
1	NRQ	D	67[A]	1	-	0/9/31/32	0/2/2/2

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	67[B]	CH6	CA1-C1	-6.27	1.42	1.51
1	A	67[B]	CH6	CA1-C1	-6.08	1.42	1.51
1	A	67[B]	CH6	C2-N3	-4.23	1.30	1.39
1	A	67[A]	NRQ	C2-N3	-4.23	1.30	1.39
1	C	67[B]	CH6	CA2-C2	-4.00	1.44	1.48
1	C	67[A]	NRQ	CA2-C2	-4.00	1.44	1.48
1	D	67[B]	CH6	C2-N3	-3.90	1.31	1.39
1	D	67[A]	NRQ	C2-N3	-3.90	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67[B]	CH6	CA1-N1	-3.42	1.32	1.49
1	D	67[B]	CH6	CA1-N1	-3.20	1.33	1.49
1	B	67[B]	CH6	C2-N3	-2.63	1.34	1.39
1	B	67[A]	NRQ	C2-N3	-2.63	1.34	1.39
1	C	67[B]	CH6	CA1-N1	-2.52	1.36	1.49
1	B	67[B]	CH6	CA1-N1	-2.51	1.36	1.49
1	C	67[B]	CH6	C2-N3	-2.35	1.34	1.39
1	C	67[A]	NRQ	C2-N3	-2.35	1.34	1.39
1	B	67[B]	CH6	CA2-C2	-2.29	1.46	1.48
1	B	67[A]	NRQ	CA2-C2	-2.29	1.46	1.48
1	B	67[A]	NRQ	C1-N3	2.10	1.43	1.38
1	D	67[B]	CH6	O2-C2	2.13	1.27	1.23
1	D	67[A]	NRQ	O2-C2	2.13	1.27	1.23
1	C	67[B]	CH6	OH-CZ	2.38	1.42	1.37
1	C	67[A]	NRQ	OH-CZ	2.38	1.42	1.37
1	C	67[B]	CH6	O2-C2	2.42	1.28	1.23
1	C	67[A]	NRQ	O2-C2	2.42	1.28	1.23
1	A	67[B]	CH6	CA3-N3	2.48	1.51	1.47
1	A	67[A]	NRQ	CA3-N3	2.48	1.51	1.47
1	A	67[B]	CH6	C1-N3	2.62	1.42	1.37
1	B	67[B]	CH6	O2-C2	2.79	1.29	1.23
1	B	67[A]	NRQ	O2-C2	2.79	1.29	1.23
1	B	67[B]	CH6	C1-N3	2.98	1.43	1.37
1	B	67[A]	NRQ	C1-N2	3.41	1.40	1.33
1	C	67[A]	NRQ	C1-N2	3.55	1.40	1.33
1	A	67[A]	NRQ	C1-N2	3.66	1.40	1.33
1	D	67[A]	NRQ	C1-N2	3.68	1.40	1.33
1	B	67[B]	CH6	C1-N2	5.07	1.40	1.32
1	C	67[B]	CH6	C1-N2	5.26	1.40	1.32
1	A	67[B]	CH6	C1-N2	5.40	1.40	1.32
1	D	67[B]	CH6	C1-N2	5.42	1.40	1.32
1	A	67[B]	CH6	CB2-CA2	12.96	1.46	1.35
1	A	67[A]	NRQ	CB2-CA2	12.96	1.46	1.35
1	B	67[B]	CH6	CB2-CA2	13.48	1.47	1.35
1	B	67[A]	NRQ	CB2-CA2	13.48	1.47	1.35
1	C	67[B]	CH6	CB2-CA2	13.62	1.47	1.35
1	C	67[A]	NRQ	CB2-CA2	13.62	1.47	1.35
1	D	67[B]	CH6	CB2-CA2	15.28	1.48	1.35
1	D	67[A]	NRQ	CB2-CA2	15.28	1.48	1.35

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	67[B]	CH6	O2-C2-CA2	-13.05	123.90	130.95
1	C	67[A]	NRQ	O2-C2-CA2	-13.05	123.90	130.95
1	D	67[B]	CH6	O2-C2-CA2	-10.44	125.31	130.95
1	D	67[A]	NRQ	O2-C2-CA2	-10.44	125.31	130.95
1	A	67[B]	CH6	O2-C2-CA2	-9.28	125.94	130.95
1	A	67[A]	NRQ	O2-C2-CA2	-9.28	125.94	130.95
1	B	67[B]	CH6	O2-C2-CA2	-8.58	126.31	130.95
1	B	67[A]	NRQ	O2-C2-CA2	-8.58	126.31	130.95
1	A	67[B]	CH6	CG2-CB2-CA2	-6.06	122.34	130.22
1	A	67[A]	NRQ	CG2-CB2-CA2	-6.06	122.34	130.22
1	C	67[B]	CH6	CB1-CA1-N1	-5.87	97.50	109.81
1	A	67[B]	CH6	CB1-CA1-N1	-5.81	97.63	109.81
1	B	67[B]	CH6	CG2-CB2-CA2	-5.43	123.16	130.22
1	B	67[A]	NRQ	CG2-CB2-CA2	-5.43	123.16	130.22
1	D	67[B]	CH6	CB1-CA1-N1	-4.84	99.67	109.81
1	D	67[B]	CH6	CA3-N3-C2	-4.72	116.30	123.99
1	D	67[A]	NRQ	CA3-N3-C2	-4.72	116.30	123.99
1	B	67[B]	CH6	CB2-CA2-C2	-4.24	116.14	122.36
1	B	67[A]	NRQ	CB2-CA2-C2	-4.24	116.14	122.36
1	A	67[B]	CH6	CA3-N3-C2	-3.99	117.50	123.99
1	A	67[A]	NRQ	CA3-N3-C2	-3.99	117.50	123.99
1	D	67[B]	CH6	CG2-CB2-CA2	-3.96	125.08	130.22
1	D	67[A]	NRQ	CG2-CB2-CA2	-3.96	125.08	130.22
1	B	67[B]	CH6	CA3-N3-C2	-3.56	118.19	123.99
1	B	67[A]	NRQ	CA3-N3-C2	-3.56	118.19	123.99
1	C	67[A]	NRQ	CB1-CG1-SD	-3.55	104.16	112.88
1	C	67[B]	CH6	CG2-CB2-CA2	-3.06	126.24	130.22
1	C	67[A]	NRQ	CG2-CB2-CA2	-3.06	126.24	130.22
1	A	67[B]	CH6	CA1-C1-N2	-3.02	116.84	123.38
1	D	67[B]	CH6	CB2-CA2-C2	-3.00	117.96	122.36
1	D	67[A]	NRQ	CB2-CA2-C2	-3.00	117.96	122.36
1	C	67[B]	CH6	CB2-CA2-C2	-3.00	117.96	122.36
1	C	67[A]	NRQ	CB2-CA2-C2	-3.00	117.96	122.36
1	A	67[A]	NRQ	CB1-CG1-SD	-2.65	106.38	112.88
1	C	67[A]	NRQ	N3-C1-N2	-2.44	110.50	113.26
1	C	67[B]	CH6	C2-CA2-N2	-2.39	107.00	108.91
1	C	67[A]	NRQ	C2-CA2-N2	-2.39	107.00	108.91
1	D	67[B]	CH6	CE-SD-CG1	-2.36	92.31	100.37
1	D	67[A]	NRQ	CE-SD-CG1	-2.36	92.31	100.37
1	C	67[B]	CH6	CE1-CD1-CG2	-2.35	118.35	121.29
1	C	67[A]	NRQ	CE1-CD1-CG2	-2.35	118.35	121.29
1	B	67[B]	CH6	CB1-CG1-SD	-2.23	103.78	113.17
1	D	67[B]	CH6	CA1-C1-N2	-2.21	118.59	123.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67[A]	NRQ	N3-C1-N2	-2.15	110.82	113.26
1	A	67[B]	CH6	CE1-CD1-CG2	-2.14	118.61	121.29
1	A	67[A]	NRQ	CE1-CD1-CG2	-2.14	118.61	121.29
1	A	67[B]	CH6	CD2-CG2-CB2	-2.08	114.12	121.23
1	A	67[A]	NRQ	CD2-CG2-CB2	-2.08	114.12	121.23
1	A	67[A]	NRQ	N3-C1-N2	-2.01	110.99	113.26
1	C	67[B]	CH6	CD1-CE1-CZ	2.03	122.21	119.87
1	C	67[A]	NRQ	CD1-CE1-CZ	2.03	122.21	119.87
1	A	67[B]	CH6	CD1-CE1-CZ	2.39	122.63	119.87
1	A	67[A]	NRQ	CD1-CE1-CZ	2.39	122.63	119.87
1	B	67[A]	NRQ	CB1-CA1-N1	2.41	129.36	124.94
1	C	67[B]	CH6	CA3-N3-C1	2.66	130.45	127.36
1	B	67[B]	CH6	CB2-CA2-N2	2.67	133.45	128.67
1	B	67[A]	NRQ	CB2-CA2-N2	2.67	133.45	128.67
1	D	67[B]	CH6	CB2-CA2-N2	3.16	134.31	128.67
1	D	67[A]	NRQ	CB2-CA2-N2	3.16	134.31	128.67
1	C	67[B]	CH6	CB2-CA2-N2	3.56	135.03	128.67
1	C	67[A]	NRQ	CB2-CA2-N2	3.56	135.03	128.67
1	A	67[B]	CH6	C3-CA3-N3	3.72	121.14	113.00
1	A	67[A]	NRQ	C3-CA3-N3	3.72	121.14	113.00
1	D	67[B]	CH6	C3-CA3-N3	4.24	122.28	113.00
1	D	67[A]	NRQ	C3-CA3-N3	4.24	122.28	113.00
1	B	67[B]	CH6	C3-CA3-N3	5.60	125.27	113.00
1	B	67[A]	NRQ	C3-CA3-N3	5.60	125.27	113.00
1	B	67[B]	CH6	CA3-N3-C1	5.69	133.96	127.36
1	B	67[B]	CH6	CA2-C2-N3	6.79	106.80	103.40
1	B	67[A]	NRQ	CA2-C2-N3	6.79	106.80	103.40
1	C	67[B]	CH6	C3-CA3-N3	7.09	128.52	113.00
1	C	67[A]	NRQ	C3-CA3-N3	7.09	128.52	113.00
1	A	67[B]	CH6	CA3-N3-C1	7.10	135.60	127.36
1	D	67[B]	CH6	CA3-N3-C1	8.67	137.42	127.36
1	A	67[B]	CH6	CA2-C2-N3	10.10	108.46	103.40
1	A	67[A]	NRQ	CA2-C2-N3	10.10	108.46	103.40
1	D	67[B]	CH6	CA2-C2-N3	11.97	109.40	103.40
1	D	67[A]	NRQ	CA2-C2-N3	11.97	109.40	103.40
1	C	67[B]	CH6	CA2-C2-N3	12.56	109.69	103.40
1	C	67[A]	NRQ	CA2-C2-N3	12.56	109.69	103.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	67[A]	NRQ	1	0
1	B	67[A]	NRQ	1	0
1	C	67[A]	NRQ	2	0
1	D	67[A]	NRQ	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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, 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	215/243 (88%)	0.28	14 (6%) 22 24	19, 28, 41, 61	13 (6%)
1	B	214/243 (88%)	0.44	17 (7%) 15 17	21, 32, 47, 62	20 (9%)
1	C	214/243 (88%)	0.38	11 (5%) 32 34	21, 34, 48, 65	23 (10%)
1	D	215/243 (88%)	0.28	8 (3%) 45 50	20, 30, 46, 73	20 (9%)
All	All	858/972 (88%)	0.34	50 (5%) 26 28	19, 31, 47, 73	76 (8%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	MET	5.5
1	C	6	ALA	5.1
1	C	222	SER	4.2
1	B	222	SER	4.0
1	A	105	VAL	3.7
1	B	199[A]	LEU	3.7
1	A	60	ILE	3.7
1	A	6	ALA	3.6
1	B	107	VAL	3.5
1	B	169	ASP	3.3
1	A	107	VAL	3.3
1	C	199	LEU	3.1
1	B	93	TRP	3.0
1	D	5	MET	3.0
1	A	124	LEU	3.0
1	A	61	LEU	2.9
1	D	124	LEU	2.9
1	A	222	SER	2.9
1	D	107	VAL	2.8
1	C	169	ASP	2.8
1	B	124	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	6	ALA	2.8
1	A	104[A]	VAL	2.7
1	C	170	GLY	2.7
1	B	170	GLY	2.6
1	B	104[A]	VAL	2.6
1	B	106	THR	2.6
1	C	124	LEU	2.6
1	B	96	VAL	2.5
1	C	137	GLN	2.5
1	C	93	TRP	2.5
1	B	168	LYS	2.4
1	B	105	VAL	2.4
1	B	95	ARG	2.4
1	D	186	PRO	2.4
1	D	96	VAL	2.4
1	A	97	MET	2.4
1	A	96	VAL	2.3
1	A	106	THR	2.3
1	C	132	ASP	2.2
1	D	60	ILE	2.2
1	D	222	SER	2.1
1	A	65[A]	PHE	2.1
1	B	13	ARG	2.1
1	D	93	TRP	2.1
1	A	22	VAL	2.0
1	B	186	PRO	2.0
1	C	107	VAL	2.0
1	B	132	ASP	2.0
1	C	105	VAL	2.0

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

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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	CH6	A	67[B]	23/24	0.94	0.12	-	25,34,47,53	23
1	CH6	D	67[B]	23/24	0.94	0.12	-	26,34,49,52	23

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	CH6	B	67[B]	23/24	0.93	0.13	-	26,34,50,55	23
1	CH6	C	67[B]	23/24	0.89	0.14	-	30,39,52,62	23
1	NRQ	A	67[A]	23/24	0.94	0.11	-	25,34,47,53	23
1	NRQ	C	67[A]	23/24	0.89	0.14	-	30,39,52,62	23
1	NRQ	B	67[A]	23/24	0.93	0.13	-	26,33,50,55	23
1	NRQ	D	67[A]	23/24	0.94	0.12	-	26,35,49,52	23

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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.