



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 08:49 pm GMT

PDB ID : 3V8E  
Title : Crystal structure of the yeast nicotinamidase Pnc1p bound to the inhibitor nicotinaldehyde  
Authors : Hoadley, K.A.; Smith, B.C.; Denu, J.M.; Keck, J.L.  
Deposited on : 2011-12-22  
Resolution : 2.71 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

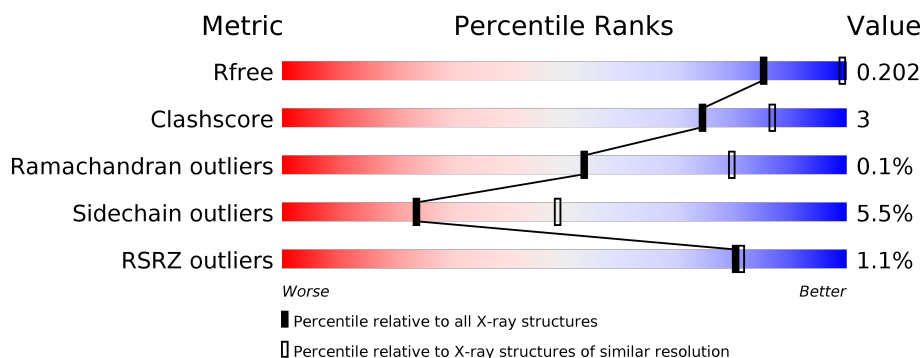
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.71 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.



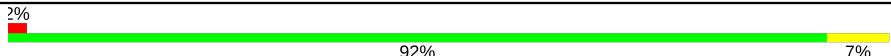
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	2885 (2.74-2.70)
Clashscore	122126	3205 (2.74-2.70)
Ramachandran outliers	120053	3157 (2.74-2.70)
Sidechain outliers	120020	3158 (2.74-2.70)
RSRZ outliers	108989	2802 (2.74-2.70)

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	216	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>12%</div> <div>.</div> </div> </div>
1	B	216	<div> <div>84%</div> <div>13%</div> <div>.</div> </div>
1	C	216	<div> <div>90%</div> <div>9%</div> <div>.</div> </div>
1	D	216	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div>.</div> </div> </div>
1	E	216	<div> <div>90%</div> <div>8%</div> <div>.</div> </div>
1	F	216	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	216	 A horizontal bar chart showing the quality of chain G. The bar is divided into three segments: a small red segment at the beginning labeled '2%', a large green segment in the middle labeled '92%', and a small yellow segment at the end labeled '7%'.

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12745 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 Nicotinamidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	1	0
			1777	1132	300	338	7			
1	B	216	Total	C	N	O	S	0	1	0
			1777	1132	300	338	7			
1	C	216	Total	C	N	O	S	0	1	0
			1777	1132	300	338	7			
1	D	216	Total	C	N	O	S	0	1	0
			1777	1132	300	338	7			
1	E	216	Total	C	N	O	S	0	1	0
			1777	1132	300	338	7			
1	F	216	Total	C	N	O	S	0	1	0
			1777	1132	300	338	7			
1	G	216	Total	C	N	O	S	0	1	0
			1777	1132	300	338	7			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total 1	Mg 1	0	0
3	D	1	Total 1	Mg 1	0	0
3	E	1	Total 1	Mg 1	0	0
3	B	1	Total 1	Mg 1	0	0
3	C	1	Total 1	Mg 1	0	0
3	A	1	Total 1	Mg 1	0	0
3	F	1	Total 1	Mg 1	0	0

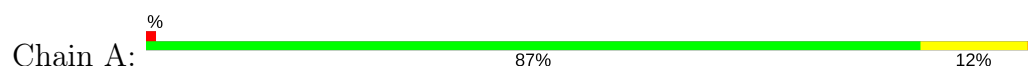
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	50	Total 50	O 50	0	0
4	B	130	Total 130	O 130	0	0
4	C	37	Total 37	O 37	0	0
4	D	26	Total 26	O 26	0	0
4	E	26	Total 26	O 26	0	0
4	F	13	Total 13	O 13	0	0
4	G	10	Total 10	O 10	0	0

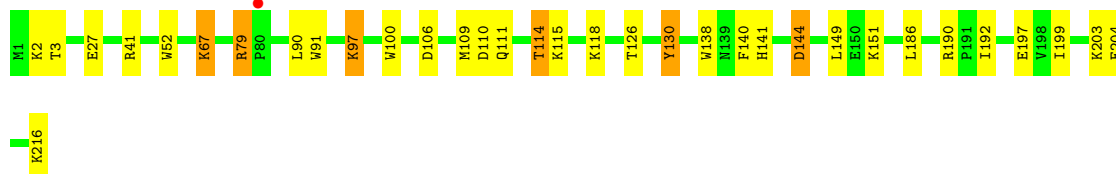
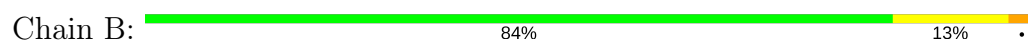
### 3 Residue-property plots

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

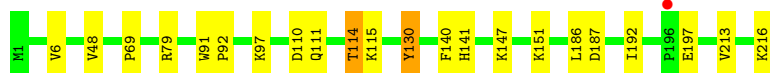
#### • Molecule 1: Nicotinamidase



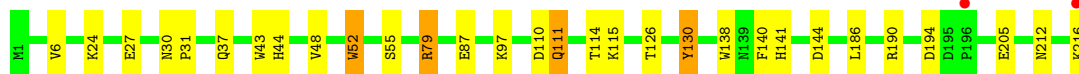
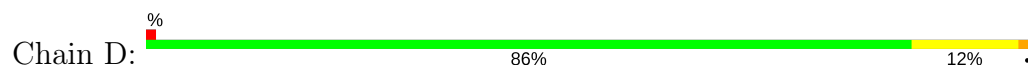
#### • Molecule 1: Nicotinamidase



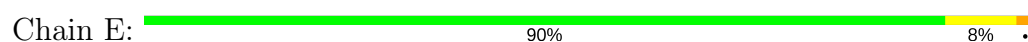
#### • Molecule 1: Nicotinamidase



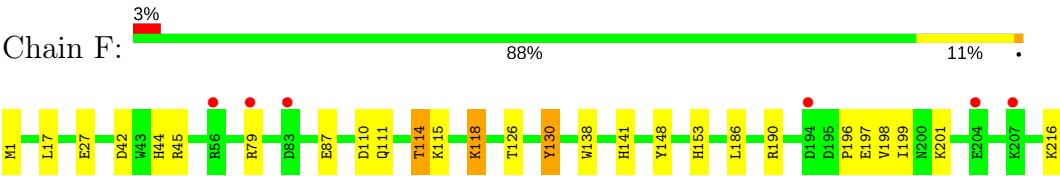
#### • Molecule 1: Nicotinamidase



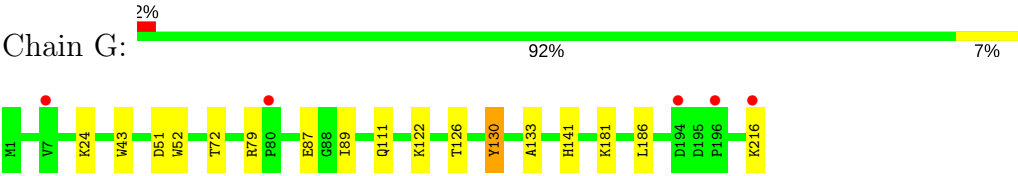
#### • Molecule 1: Nicotinamidase



#### • Molecule 1: Nicotinamidase



• Molecule 1: Nicotinamidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	298.72Å 298.72Å 112.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.71 29.87 – 2.71	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-2.71) 99.8 (29.87-2.71)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.07 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.181 , 0.203 0.180 , 0.202	Depositor DCC
$R_{free}$ test set	5058 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.7	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 36.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12745	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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, 0.333 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: ZN, MG, JJJ

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	0.62	3/1811 (0.2%)	0.67	0/2460
1	B	0.60	3/1811 (0.2%)	0.67	0/2460
1	C	0.59	1/1811 (0.1%)	0.63	0/2460
1	D	0.56	3/1811 (0.2%)	0.61	1/2460 (0.0%)
1	E	0.56	0/1811	0.62	0/2460
1	F	0.54	1/1811 (0.1%)	0.59	0/2460
1	G	0.55	2/1811 (0.1%)	0.56	0/2460
All	All	0.58	13/12677 (0.1%)	0.62	1/17220 (0.0%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	91	TRP	CD2-CE2	5.80	1.48	1.41
1	B	100	TRP	CD2-CE2	5.66	1.48	1.41
1	A	100	TRP	CD2-CE2	5.34	1.47	1.41
1	C	91	TRP	CD2-CE2	5.28	1.47	1.41
1	B	138	TRP	CD2-CE2	5.25	1.47	1.41
1	D	52	TRP	CD2-CE2	5.25	1.47	1.41
1	G	43	TRP	CD2-CE2	5.24	1.47	1.41
1	G	52	TRP	CD2-CE2	5.20	1.47	1.41
1	D	138	TRP	CD2-CE2	5.11	1.47	1.41
1	A	91	TRP	CD2-CE2	5.07	1.47	1.41
1	F	138	TRP	CD2-CE2	5.05	1.47	1.41
1	A	52	TRP	CD2-CE2	5.04	1.47	1.41
1	D	43	TRP	CD2-CE2	5.03	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	144	ASP	CB-CA-C	-5.46	99.49	110.40

There are no chirality outliers.

There are no planarity outliers.

## 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	1777	0	1731	24	0
1	B	1777	0	1731	22	0
1	C	1777	0	1731	12	0
1	D	1777	0	1731	11	0
1	E	1777	0	1730	8	0
1	F	1777	0	1731	13	0
1	G	1777	0	1731	4	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
4	A	50	0	0	3	0
4	B	130	0	0	4	0
4	C	37	0	0	0	0
4	D	26	0	0	1	0
4	E	26	0	0	0	0
4	F	13	0	0	1	0
4	G	10	0	0	1	0
All	All	12745	0	12116	85	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 3.

All (85) 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)
4:A:424:HOH:O	1:C:147:LYS:HD2	1.62	0.98
1:A:166:TYR:CE2	1:A:192:ILE:HD11	2.08	0.88
1:A:130:TYR:OH	1:A:141:HIS:HD2	1.60	0.83
1:A:79:ARG:HH21	1:A:140:PHE:HB3	1.45	0.79
1:C:130:TYR:OH	1:C:141:HIS:HD2	1.65	0.79
1:A:125:LEU:HD11	1:B:109:MET:CE	2.14	0.77
1:E:110:ASP:O	1:E:114:THR:HG23	1.86	0.75
1:B:110:ASP:O	1:B:114:THR:HG23	1.89	0.73
1:D:27:GLU:HB2	1:D:190:ARG:HH12	1.54	0.72
1:D:130:TYR:OH	1:D:141:HIS:HD2	1.74	0.71
1:A:79:ARG:HB2	1:A:140:PHE:CE1	2.26	0.70
1:C:110:ASP:O	1:C:114:THR:HG23	1.93	0.69
1:E:130:TYR:OH	1:E:141:HIS:HD2	1.77	0.69
1:B:130:TYR:OH	1:B:141:HIS:HD2	1.78	0.66
1:F:130:TYR:OH	1:F:141:HIS:HD2	1.80	0.65
1:A:130:TYR:OH	1:A:141:HIS:CD2	2.46	0.64
1:A:125:LEU:HD11	1:B:109:MET:HE3	1.80	0.62
1:A:79:ARG:NH2	1:A:140:PHE:HB3	2.13	0.62
1:F:198:VAL:HA	1:F:201:LYS:HG3	1.84	0.60
1:G:130:TYR:OH	1:G:141:HIS:HD2	1.85	0.60
1:E:151:LYS:HE3	1:F:17:LEU:HD23	1.84	0.60
1:B:67:LYS:HG2	1:B:90:LEU:HD12	1.83	0.59
1:A:141:HIS:HB2	1:B:109:MET:HE1	1.84	0.59
1:D:37:GLN:HG3	1:D:111:GLN:OE1	2.04	0.58
1:B:2:LYS:CE	1:B:41:ARG:O	2.54	0.56
1:A:125:LEU:CD1	1:B:109:MET:HE3	2.37	0.55
1:F:27:GLU:HB2	1:F:190:ARG:HH12	1.72	0.54
1:C:114:THR:HG22	4:D:410:HOH:O	2.07	0.54
1:A:166:TYR:HE2	1:A:192:ILE:HD11	1.69	0.53
1:B:115:LYS:HD2	4:B:515:HOH:O	2.09	0.53
1:D:110:ASP:O	1:D:114:THR:HG23	2.09	0.53
1:F:196:PRO:O	1:F:199:ILE:HG22	2.09	0.52
1:B:2:LYS:HE2	1:B:41:ARG:O	2.10	0.52
1:C:130:TYR:OH	1:C:141:HIS:CD2	2.56	0.51
1:G:126:THR:HG22	4:G:407:HOH:O	2.10	0.51
1:D:52:TRP:CE2	1:D:97:LYS:HB3	2.45	0.51
1:F:44:HIS:O	1:F:45:ARG:HD2	2.11	0.51
1:A:141:HIS:ND1	1:B:109:MET:CE	2.74	0.50
1:A:111:GLN:HG3	1:A:115:LYS:HD2	1.91	0.50
1:F:118:LYS:HD2	1:F:148:TYR:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:27:GLU:OE1	1:F:190:ARG:NH1	2.43	0.50
1:E:79:ARG:HB2	1:E:140:PHE:CE1	2.47	0.50
1:B:118:LYS:NZ	1:B:144:ASP:OD2	2.37	0.49
1:D:37:GLN:CG	1:D:111:GLN:OE1	2.60	0.49
1:F:118:LYS:HE3	4:F:402:HOH:O	2.12	0.49
1:C:187:ASP:OD2	1:C:216:LYS:HD3	2.14	0.48
1:D:44:HIS:HE1	1:E:195:ASP:OD2	1.96	0.47
1:A:137:ILE:HD11	4:B:440:HOH:O	2.13	0.47
1:F:110:ASP:O	1:F:114:THR:HG23	2.14	0.47
1:A:2:LYS:HE2	4:A:447:HOH:O	2.14	0.47
1:A:141:HIS:HE1	1:B:106:ASP:OD1	1.98	0.46
1:A:166:TYR:CD2	1:A:192:ILE:HD11	2.50	0.46
1:B:114:THR:HG22	4:B:502:HOH:O	2.16	0.46
1:B:199:ILE:O	1:B:203:LYS:HB2	2.16	0.46
1:A:79:ARG:HH21	1:A:140:PHE:CB	2.21	0.46
1:D:79:ARG:HD3	1:D:140:PHE:CD1	2.51	0.46
1:G:122:LYS:HD3	1:G:133:ALA:HA	1.96	0.46
1:E:122:LYS:HD3	1:E:133:ALA:HA	1.97	0.45
1:A:110:ASP:O	1:A:114:THR:HG23	2.17	0.45
1:D:30:ASN:HB2	1:D:31:PRO:HD3	1.99	0.45
1:G:72:THR:HG22	1:G:89:ILE:HD13	1.99	0.45
1:A:141:HIS:ND1	1:B:109:MET:HE1	2.33	0.44
1:F:27:GLU:HB2	1:F:190:ARG:NH1	2.33	0.44
1:F:44:HIS:O	1:F:45:ARG:CD	2.66	0.44
1:B:3:THR:HG21	1:B:149:LEU:CD2	2.48	0.43
1:C:69:PRO:HB3	1:C:92:PRO:HD3	2.00	0.43
1:B:126:THR:HG22	4:B:523:HOH:O	2.17	0.43
1:D:27:GLU:HB2	1:D:190:ARG:NH1	2.28	0.43
1:A:159:ILE:CD1	1:A:172:ALA:HA	2.49	0.43
1:B:2:LYS:HE3	1:B:41:ARG:O	2.19	0.43
1:C:186:LEU:HA	1:C:186:LEU:HD23	1.86	0.42
1:C:79:ARG:NH2	1:C:140:PHE:HB3	2.33	0.42
1:D:6:VAL:HB	1:D:48:VAL:HG12	2.01	0.42
1:A:193:SER:C	1:A:195:ASP:H	2.22	0.42
1:B:79:ARG:HB2	1:B:140:PHE:CE1	2.54	0.42
1:C:6:VAL:HB	1:C:48:VAL:HG12	2.01	0.42
1:A:97:LYS:HD2	4:A:445:HOH:O	2.20	0.42
1:C:186:LEU:HG	1:C:213:VAL:CG1	2.49	0.42
1:F:1:MET:HG3	1:F:153:HIS:HB2	2.01	0.42
1:E:27:GLU:OE1	1:E:190:ARG:NH1	2.53	0.42
1:A:140:PHE:HD2	1:A:140:PHE:HA	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:GLU:OE1	1:B:190:ARG:NH1	2.54	0.41
1:C:130:TYR:HH	1:C:141:HIS:HD2	1.63	0.41
1:E:129[B]:GLU:HB2	1:E:137:ILE:HD13	2.02	0.41
1:B:52:TRP:CE2	1:B:97:LYS:HB3	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	214/216 (99%)	205 (96%)	8 (4%)	1 (0%)	31	57
1	B	214/216 (99%)	202 (94%)	12 (6%)	0	100	100
1	C	214/216 (99%)	201 (94%)	13 (6%)	0	100	100
1	D	214/216 (99%)	202 (94%)	12 (6%)	0	100	100
1	E	214/216 (99%)	205 (96%)	9 (4%)	0	100	100
1	F	214/216 (99%)	202 (94%)	12 (6%)	0	100	100
1	G	214/216 (99%)	202 (94%)	12 (6%)	0	100	100
All	All	1498/1512 (99%)	1419 (95%)	78 (5%)	1 (0%)	53	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	ASP

### 5.3.2 Protein sidechains [i](#)

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	199/198 (100%)	189 (95%)	10 (5%)	27	53
1	B	199/198 (100%)	186 (94%)	13 (6%)	19	41
1	C	199/198 (100%)	191 (96%)	8 (4%)	34	63
1	D	199/198 (100%)	186 (94%)	13 (6%)	19	41
1	E	199/198 (100%)	188 (94%)	11 (6%)	24	49
1	F	199/198 (100%)	187 (94%)	12 (6%)	21	45
1	G	199/198 (100%)	190 (96%)	9 (4%)	30	58
All	All	1393/1386 (100%)	1317 (94%)	76 (6%)	24	49

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LYS
1	A	26	GLU
1	A	111	GLN
1	A	126	THR
1	A	130	TYR
1	A	151	LYS
1	A	186	LEU
1	A	192	ILE
1	A	204	GLU
1	A	210	ASN
1	B	67	LYS
1	B	79	ARG
1	B	97	LYS
1	B	111	GLN
1	B	114	THR
1	B	130	TYR
1	B	144	ASP
1	B	151	LYS
1	B	186	LEU
1	B	192	ILE
1	B	197	GLU
1	B	204	GLU
1	B	216	LYS
1	C	97	LYS
1	C	111	GLN
1	C	114	THR

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Mol	Chain	Res	Type
1	C	115	LYS
1	C	130	TYR
1	C	151	LYS
1	C	192	ILE
1	C	197	GLU
1	D	24	LYS
1	D	55	SER
1	D	79	ARG
1	D	87	GLU
1	D	111	GLN
1	D	115	LYS
1	D	126	THR
1	D	130	TYR
1	D	186	LEU
1	D	194	ASP
1	D	205	GLU
1	D	212	ASN
1	D	216	LYS
1	E	62	LYS
1	E	79	ARG
1	E	111	GLN
1	E	114	THR
1	E	130	TYR
1	E	151	LYS
1	E	186	LEU
1	E	192	ILE
1	E	201	LYS
1	E	210	ASN
1	E	212	ASN
1	F	42	ASP
1	F	79	ARG
1	F	87	GLU
1	F	111	GLN
1	F	114	THR
1	F	115	LYS
1	F	118	LYS
1	F	126	THR
1	F	130	TYR
1	F	186	LEU
1	F	197	GLU
1	F	216	LYS
1	G	24	LYS

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Mol	Chain	Res	Type
1	G	51	ASP
1	G	79	ARG
1	G	87	GLU
1	G	111	GLN
1	G	130	TYR
1	G	181	LYS
1	G	186	LEU
1	G	216	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	141	HIS
1	A	209	HIS
1	B	141	HIS
1	C	37	GLN
1	C	141	HIS
1	C	212	ASN
1	D	37	GLN
1	D	141	HIS
1	D	212	ASN
1	E	37	GLN
1	E	103	GLN
1	E	107	GLN
1	E	141	HIS
1	E	209	HIS
1	F	37	GLN
1	F	111	GLN
1	F	141	HIS
1	F	209	HIS
1	G	37	GLN
1	G	103	GLN
1	G	111	GLN
1	G	141	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

7 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	JJJ	A	167	1,2	14,14,15	1.28	2 (14%)	13,17,19	2.71	5 (38%)
1	JJJ	B	167	1,2	14,14,15	1.24	1 (7%)	13,17,19	2.96	6 (46%)
1	JJJ	C	167	1	14,14,15	1.19	1 (7%)	13,17,19	2.63	5 (38%)
1	JJJ	D	167	1	14,14,15	1.30	1 (7%)	13,17,19	2.86	5 (38%)
1	JJJ	E	167	1,2	14,14,15	1.47	1 (7%)	13,17,19	2.42	5 (38%)
1	JJJ	F	167	1	14,14,15	1.37	1 (7%)	13,17,19	2.27	4 (30%)
1	JJJ	G	167	1	14,14,15	1.30	1 (7%)	13,17,19	2.61	4 (30%)

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	JJJ	A	167	1,2	-	0/9/11/13	0/1/1/1
1	JJJ	B	167	1,2	-	0/9/11/13	0/1/1/1
1	JJJ	C	167	1	-	0/9/11/13	0/1/1/1
1	JJJ	D	167	1	-	0/9/11/13	0/1/1/1
1	JJJ	E	167	1,2	-	0/9/11/13	0/1/1/1
1	JJJ	F	167	1	-	0/9/11/13	0/1/1/1
1	JJJ	G	167	1	-	0/9/11/13	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	167	JJJ	C7-SG	-4.54	1.67	1.76
1	F	167	JJJ	C7-SG	-4.25	1.68	1.76
1	G	167	JJJ	C7-SG	-3.96	1.68	1.76
1	D	167	JJJ	C7-SG	-3.95	1.68	1.76
1	C	167	JJJ	C7-SG	-3.74	1.69	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	167	JJJ	C7-SG	-3.69	1.69	1.76
1	A	167	JJJ	C7-SG	-3.35	1.70	1.76
1	A	167	JJJ	CA-C	2.27	1.53	1.50

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	167	JJJ	C3-C2-N1	-2.93	119.07	123.47
1	C	167	JJJ	C3-C2-N1	-2.58	119.59	123.47
1	D	167	JJJ	O7-C7-C3	-2.51	115.84	122.14
1	D	167	JJJ	C3-C2-N1	-2.42	119.83	123.47
1	A	167	JJJ	C3-C2-N1	-2.37	119.91	123.47
1	B	167	JJJ	O7-C7-C3	-2.34	116.28	122.14
1	E	167	JJJ	C3-C2-N1	-2.33	119.96	123.47
1	F	167	JJJ	C3-C2-N1	-2.22	120.13	123.47
1	C	167	JJJ	O7-C7-C3	-2.20	116.62	122.14
1	A	167	JJJ	O7-C7-C3	-2.17	116.70	122.14
1	G	167	JJJ	C3-C2-N1	-2.07	120.35	123.47
1	B	167	JJJ	C4-C3-C2	2.00	119.95	117.65
1	E	167	JJJ	C4-C3-C2	2.13	120.10	117.65
1	E	167	JJJ	C6-N1-C2	2.17	120.61	116.83
1	G	167	JJJ	C6-N1-C2	2.43	121.08	116.83
1	F	167	JJJ	C6-N1-C2	2.67	121.48	116.83
1	C	167	JJJ	C6-N1-C2	2.75	121.62	116.83
1	B	167	JJJ	C6-N1-C2	2.86	121.82	116.83
1	D	167	JJJ	C6-N1-C2	2.90	121.88	116.83
1	E	167	JJJ	C3-C7-SG	2.99	121.21	114.99
1	A	167	JJJ	C6-N1-C2	3.18	122.37	116.83
1	G	167	JJJ	C3-C7-SG	3.43	122.14	114.99
1	B	167	JJJ	C3-C7-SG	3.47	122.22	114.99
1	C	167	JJJ	C3-C7-SG	3.58	122.45	114.99
1	A	167	JJJ	C3-C7-SG	3.66	122.61	114.99
1	F	167	JJJ	C3-C7-SG	3.68	122.66	114.99
1	D	167	JJJ	C3-C7-SG	4.25	123.84	114.99
1	F	167	JJJ	CB-SG-C7	5.43	106.73	99.84
1	E	167	JJJ	CB-SG-C7	6.65	108.27	99.84
1	C	167	JJJ	CB-SG-C7	7.13	108.89	99.84
1	A	167	JJJ	CB-SG-C7	7.42	109.25	99.84
1	G	167	JJJ	CB-SG-C7	7.45	109.29	99.84
1	D	167	JJJ	CB-SG-C7	7.73	109.64	99.84
1	B	167	JJJ	CB-SG-C7	8.41	110.50	99.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 14 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, 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	215/216 (99%)	-0.45	2 (0%) 84 85	24, 34, 61, 73	0
1	B	215/216 (99%)	-0.37	1 (0%) 90 92	23, 38, 71, 87	0
1	C	215/216 (99%)	-0.36	1 (0%) 90 92	27, 44, 83, 114	0
1	D	215/216 (99%)	-0.22	2 (0%) 84 85	40, 58, 95, 124	0
1	E	215/216 (99%)	-0.30	0 100 100	30, 50, 77, 96	0
1	F	215/216 (99%)	-0.01	6 (2%) 53 54	50, 75, 113, 137	0
1	G	215/216 (99%)	0.01	5 (2%) 60 61	55, 76, 116, 141	0
All	All	1505/1512 (99%)	-0.24	17 (1%) 80 81	23, 54, 100, 141	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	216	LYS	3.7
1	G	194	ASP	3.2
1	G	196	PRO	3.0
1	D	196	PRO	2.9
1	F	56	ARG	2.8
1	D	216	LYS	2.7
1	F	207	LYS	2.7
1	F	83	ASP	2.5
1	B	80	PRO	2.4
1	F	79	ARG	2.4
1	C	196	PRO	2.1
1	A	216	LYS	2.1
1	A	80	PRO	2.0
1	G	80	PRO	2.0
1	F	194	ASP	2.0
1	F	204	GLU	2.0
1	G	7	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
1	JJJ	G	167	14/15	0.93	0.27	75,88,92,92	0
1	JJJ	D	167	14/15	0.94	0.25	53,63,74,74	0
1	JJJ	C	167	14/15	0.95	0.26	44,59,64,64	0
1	JJJ	E	167	14/15	0.95	0.26	48,59,68,69	0
1	JJJ	F	167	14/15	0.95	0.26	75,84,89,90	0
1	JJJ	A	167	14/15	0.97	0.23	31,42,50,50	0
1	JJJ	B	167	14/15	0.97	0.22	36,47,53,53	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	C	301	1/1	0.83	0.07	60,60,60,60	0
2	ZN	G	300	1/1	0.88	0.15	139,139,139,139	0
3	MG	F	301	1/1	0.89	0.11	62,62,62,62	0
3	MG	G	301	1/1	0.90	0.08	79,79,79,79	0
2	ZN	C	300	1/1	0.90	0.08	112,112,112,112	0
2	ZN	E	300	1/1	0.92	0.10	109,109,109,109	0
3	MG	E	301	1/1	0.92	0.09	45,45,45,45	0
3	MG	D	301	1/1	0.94	0.04	69,69,69,69	0
3	MG	B	301	1/1	0.96	0.07	43,43,43,43	0
2	ZN	A	300	1/1	0.97	0.07	84,84,84,84	0
2	ZN	B	300	1/1	0.97	0.11	95,95,95,95	0
3	MG	A	301	1/1	0.97	0.08	51,51,51,51	0
2	ZN	F	300	1/1	0.97	0.17	142,142,142,142	0
2	ZN	D	300	1/1	0.99	0.05	103,103,103,103	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.