



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 7, 2017 – 05:08 PM EST

PDB ID : 5UGT  
Title : Crystal structure of M. tuberculosis InhA inhibited by PT504  
Authors : Eltschkner, S.; Pschibul, A.; Spagnuolo, L.A.; Yu, W.; Tonge, P.J.; Kisker, C.  
Deposited on : 2017-01-10  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
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) : rb-20028442

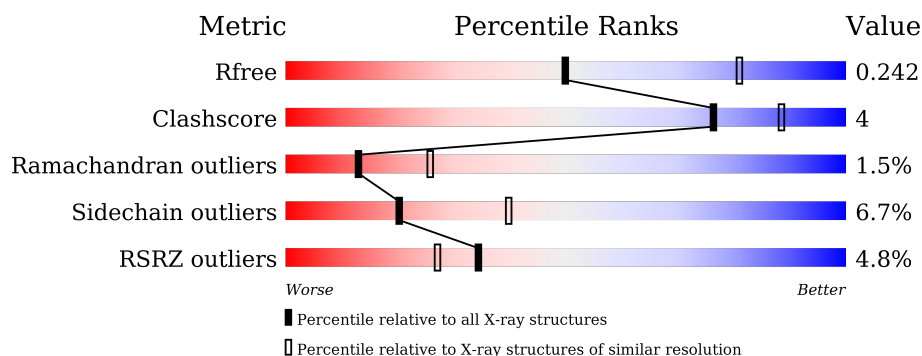
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	289	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>13%</div> <div>•</div> <div>7%</div> </div> </div>
1	B	289	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>10%</div> <div>•</div> <div>10%</div> </div> </div>
1	E	289	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>10%</div> <div>•</div> <div>7%</div> </div> </div>
1	G	289	<div> <div>8%</div> <div> <div></div> <div>80%</div> <div>8%</div> <div>•</div> <div>9%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8332 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 Enoyl-[acyl-carrier-protein] reductase [NADH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			1995	1264	348	373	10			
1	B	261	Total	C	N	O	S	0	0	0
			1952	1239	341	362	10			
1	E	268	Total	C	N	O	S	0	2	0
			2001	1268	348	375	10			
1	G	264	Total	C	N	O	S	0	1	0
			1979	1255	344	369	11			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P9WGR1
A	-18	GLY	-	expression tag	UNP P9WGR1
A	-17	SER	-	expression tag	UNP P9WGR1
A	-16	SER	-	expression tag	UNP P9WGR1
A	-15	HIS	-	expression tag	UNP P9WGR1
A	-14	HIS	-	expression tag	UNP P9WGR1
A	-13	HIS	-	expression tag	UNP P9WGR1
A	-12	HIS	-	expression tag	UNP P9WGR1
A	-11	HIS	-	expression tag	UNP P9WGR1
A	-10	HIS	-	expression tag	UNP P9WGR1
A	-9	SER	-	expression tag	UNP P9WGR1
A	-8	SER	-	expression tag	UNP P9WGR1
A	-7	GLY	-	expression tag	UNP P9WGR1
A	-6	LEU	-	expression tag	UNP P9WGR1
A	-5	VAL	-	expression tag	UNP P9WGR1
A	-4	PRO	-	expression tag	UNP P9WGR1
A	-3	ARG	-	expression tag	UNP P9WGR1
A	-2	GLY	-	expression tag	UNP P9WGR1
A	-1	SER	-	expression tag	UNP P9WGR1
A	0	HIS	-	expression tag	UNP P9WGR1
B	-19	MET	-	initiating methionine	UNP P9WGR1

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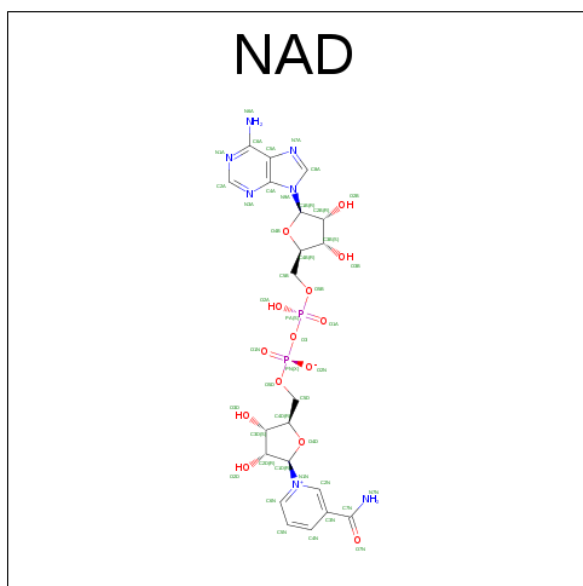
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP P9WGR1
B	-17	SER	-	expression tag	UNP P9WGR1
B	-16	SER	-	expression tag	UNP P9WGR1
B	-15	HIS	-	expression tag	UNP P9WGR1
B	-14	HIS	-	expression tag	UNP P9WGR1
B	-13	HIS	-	expression tag	UNP P9WGR1
B	-12	HIS	-	expression tag	UNP P9WGR1
B	-11	HIS	-	expression tag	UNP P9WGR1
B	-10	HIS	-	expression tag	UNP P9WGR1
B	-9	SER	-	expression tag	UNP P9WGR1
B	-8	SER	-	expression tag	UNP P9WGR1
B	-7	GLY	-	expression tag	UNP P9WGR1
B	-6	LEU	-	expression tag	UNP P9WGR1
B	-5	VAL	-	expression tag	UNP P9WGR1
B	-4	PRO	-	expression tag	UNP P9WGR1
B	-3	ARG	-	expression tag	UNP P9WGR1
B	-2	GLY	-	expression tag	UNP P9WGR1
B	-1	SER	-	expression tag	UNP P9WGR1
B	0	HIS	-	expression tag	UNP P9WGR1
E	-19	MET	-	initiating methionine	UNP P9WGR1
E	-18	GLY	-	expression tag	UNP P9WGR1
E	-17	SER	-	expression tag	UNP P9WGR1
E	-16	SER	-	expression tag	UNP P9WGR1
E	-15	HIS	-	expression tag	UNP P9WGR1
E	-14	HIS	-	expression tag	UNP P9WGR1
E	-13	HIS	-	expression tag	UNP P9WGR1
E	-12	HIS	-	expression tag	UNP P9WGR1
E	-11	HIS	-	expression tag	UNP P9WGR1
E	-10	HIS	-	expression tag	UNP P9WGR1
E	-9	SER	-	expression tag	UNP P9WGR1
E	-8	SER	-	expression tag	UNP P9WGR1
E	-7	GLY	-	expression tag	UNP P9WGR1
E	-6	LEU	-	expression tag	UNP P9WGR1
E	-5	VAL	-	expression tag	UNP P9WGR1
E	-4	PRO	-	expression tag	UNP P9WGR1
E	-3	ARG	-	expression tag	UNP P9WGR1
E	-2	GLY	-	expression tag	UNP P9WGR1
E	-1	SER	-	expression tag	UNP P9WGR1
E	0	HIS	-	expression tag	UNP P9WGR1
G	-19	MET	-	initiating methionine	UNP P9WGR1
G	-18	GLY	-	expression tag	UNP P9WGR1
G	-17	SER	-	expression tag	UNP P9WGR1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-16	SER	-	expression tag	UNP P9WGR1
G	-15	HIS	-	expression tag	UNP P9WGR1
G	-14	HIS	-	expression tag	UNP P9WGR1
G	-13	HIS	-	expression tag	UNP P9WGR1
G	-12	HIS	-	expression tag	UNP P9WGR1
G	-11	HIS	-	expression tag	UNP P9WGR1
G	-10	HIS	-	expression tag	UNP P9WGR1
G	-9	SER	-	expression tag	UNP P9WGR1
G	-8	SER	-	expression tag	UNP P9WGR1
G	-7	GLY	-	expression tag	UNP P9WGR1
G	-6	LEU	-	expression tag	UNP P9WGR1
G	-5	VAL	-	expression tag	UNP P9WGR1
G	-4	PRO	-	expression tag	UNP P9WGR1
G	-3	ARG	-	expression tag	UNP P9WGR1
G	-2	GLY	-	expression tag	UNP P9WGR1
G	-1	SER	-	expression tag	UNP P9WGR1
G	0	HIS	-	expression tag	UNP P9WGR1

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).



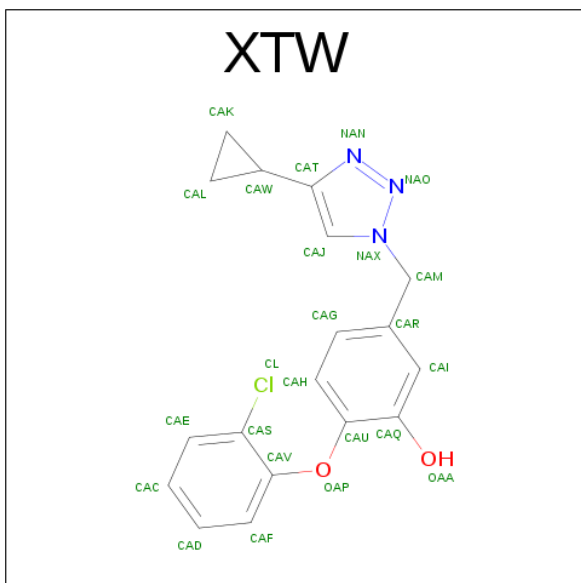
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is 2-(2-chloranylphenoxy)-5-[(4-cyclopropyl-1,2,3-triazol-1-yl)methyl]phenol (three-letter code: XTW) (formula: C<sub>18</sub>H<sub>16</sub>ClN<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			24	18	1	3	2		
3	B	1	Total	C	Cl	N	O	0	0
			24	18	1	3	2		
3	E	1	Total	C	Cl	N	O	0	0
			24	18	1	3	2		
3	G	1	Total	C	Cl	N	O	0	0
			24	18	1	3	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	48	Total	O	0	0
			48	48		
4	B	24	Total	O	0	0
			24	24		
4	E	44	Total	O	0	0
			44	44		

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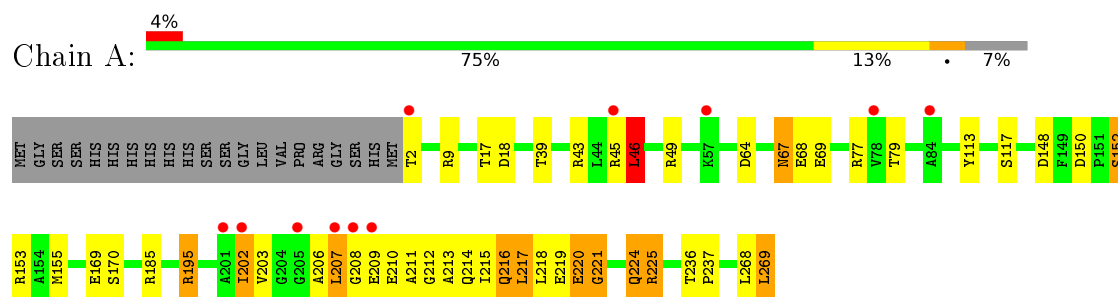
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	17	Total	O	0	0
			17	17		

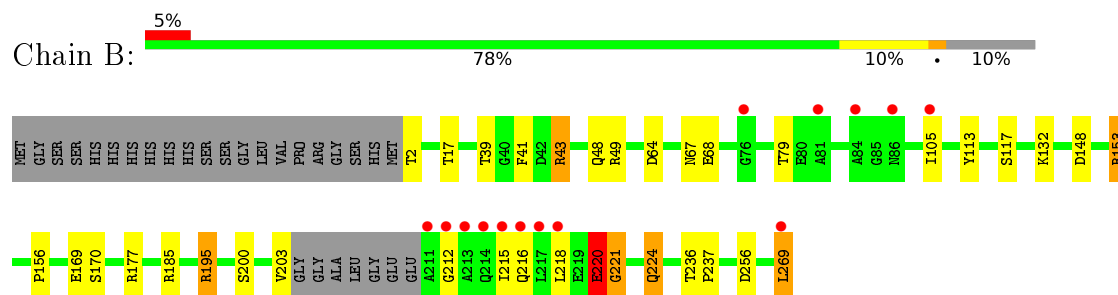
### 3 Residue-property plots [i](#)

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.

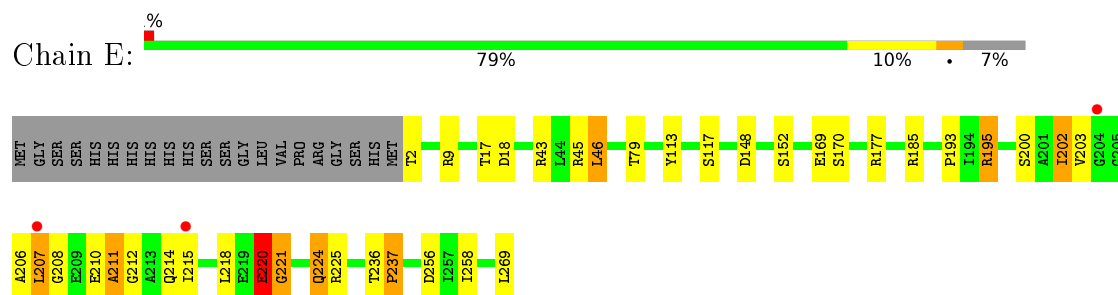
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



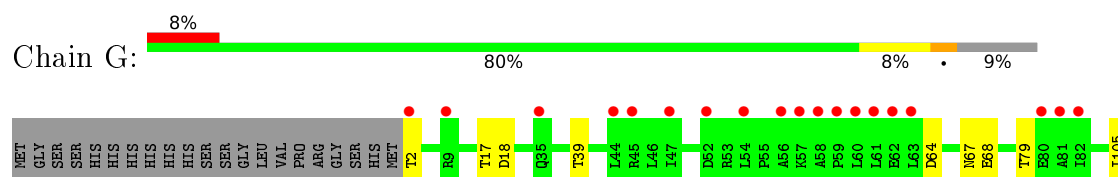
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

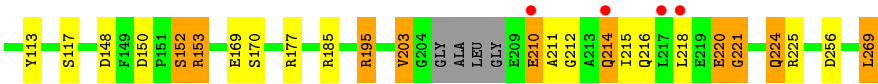


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.92Å 92.78Å 180.43Å 90.00° 97.26° 90.00°	Depositor
Resolution (Å)	46.58 – 2.60 46.58 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.58-2.60) 98.5 (46.58-2.60)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.211 , 0.239 0.212 , 0.242	Depositor DCC
$R_{free}$ test set	2159 reflections (5.19%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.3	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 41.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8332	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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: XTW, NAD

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	0.87	3/2033 (0.1%)	1.03	13/2761 (0.5%)
1	B	0.84	3/1989 (0.2%)	0.98	9/2701 (0.3%)
1	E	0.92	3/2045 (0.1%)	1.02	10/2777 (0.4%)
1	G	0.81	3/2019 (0.1%)	0.98	9/2741 (0.3%)
All	All	0.86	12/8086 (0.1%)	1.00	41/10980 (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	A	0	2
1	B	0	1
1	E	0	2
1	G	0	1
All	All	0	6

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	221	GLY	N-CA	6.63	1.55	1.46
1	G	221	GLY	N-CA	6.41	1.55	1.46
1	A	221	GLY	CA-C	5.92	1.61	1.51
1	A	221	GLY	C-O	5.78	1.32	1.23
1	G	153	ARG	NE-CZ	5.62	1.40	1.33
1	G	152	SER	CA-CB	5.62	1.61	1.52
1	E	221	GLY	N-CA	5.57	1.54	1.46
1	B	153	ARG	NE-CZ	5.46	1.40	1.33
1	E	221	GLY	CA-C	5.28	1.60	1.51
1	B	221	GLY	CA-C	5.20	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	221	GLY	C-O	5.17	1.31	1.23
1	A	153	ARG	CZ-NH2	5.09	1.39	1.33

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	153	ARG	NE-CZ-NH1	10.57	125.58	120.30
1	B	153	ARG	NE-CZ-NH1	10.53	125.57	120.30
1	A	195	ARG	NE-CZ-NH2	10.22	125.41	120.30
1	E	46	LEU	CB-CG-CD2	8.56	125.55	111.00
1	E	9	ARG	NE-CZ-NH1	-8.19	116.20	120.30
1	A	195	ARG	NE-CZ-NH1	-7.77	116.42	120.30
1	B	195	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	A	217	LEU	CB-CG-CD2	7.19	123.22	111.00
1	G	152	SER	N-CA-CB	-7.15	99.78	110.50
1	E	185	ARG	NE-CZ-NH2	6.88	123.74	120.30
1	G	177	ARG	NE-CZ-NH1	-6.81	116.90	120.30
1	E	185	ARG	NE-CZ-NH1	-6.09	117.26	120.30
1	G	195	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	G	225	ARG	CA-CB-CG	6.04	126.68	113.40
1	G	256	ASP	CB-CG-OD1	6.01	123.71	118.30
1	E	256	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	E	18	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	A	9	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	E	225	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	G	185	ARG	NE-CZ-NH2	5.76	123.18	120.30
1	B	256	ASP	CB-CG-OD1	5.70	123.42	118.30
1	B	269	LEU	CB-CG-CD2	5.66	120.61	111.00
1	B	43	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	B	185	ARG	NE-CZ-NH2	5.55	123.08	120.30
1	A	77	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	A	225	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	E	18	ASP	CB-CG-OD1	5.47	123.22	118.30
1	A	46	LEU	CB-CG-CD1	5.44	120.25	111.00
1	A	18	ASP	CB-CG-OD1	5.41	123.16	118.30
1	A	64	ASP	N-CA-C	-5.32	96.63	111.00
1	A	195	ARG	CG-CD-NE	-5.27	100.74	111.80
1	G	64	ASP	N-CA-C	-5.22	96.91	111.00
1	E	177	ARG	NE-CZ-NH2	5.21	122.90	120.30
1	A	185	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	B	64	ASP	N-CA-C	-5.17	97.04	111.00
1	A	155	MET	CG-SD-CE	5.11	108.38	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	ARG	NE-CZ-NH1	-5.11	117.75	120.30
1	B	49	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	177	ARG	NE-CZ-NH2	5.05	122.82	120.30
1	E	195	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	G	18	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	210	GLU	Peptide
1	A	220	GLU	Peptide
1	B	220	GLU	Peptide
1	E	210	GLU	Peptide
1	E	220	GLU	Peptide
1	G	220	GLU	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	1995	0	2013	24	0
1	B	1952	0	1975	13	0
1	E	2001	0	2023	19	0
1	G	1979	0	1999	12	0
2	A	44	0	26	1	0
2	B	44	0	26	1	0
2	E	44	0	26	1	0
2	G	44	0	26	0	0
3	A	24	0	0	3	0
3	B	24	0	0	1	0
3	E	24	0	0	0	0
3	G	24	0	0	1	0
4	A	48	0	0	2	0
4	B	24	0	0	1	0
4	E	44	0	0	0	0
4	G	17	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8332	0	8114	62	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 4.

All (62) 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:A:269:LEU:HD13	1:E:218:LEU:CD1	1.95	0.96
1:A:269:LEU:HD13	1:E:218:LEU:HD12	1.56	0.87
1:G:214:GLN:OE1	1:G:214:GLN:HA	1.80	0.80
1:A:214:GLN:OE1	1:A:214:GLN:HA	1.83	0.76
1:A:269:LEU:HD13	1:E:218:LEU:HD13	1.75	0.67
1:E:46:LEU:H	1:E:46:LEU:HD12	1.61	0.66
1:B:2:THR:HA	1:E:2:THR:OG1	1.95	0.66
1:G:203:VAL:HG11	1:G:211:ALA:HB3	1.77	0.65
1:G:218:LEU:HD23	3:G:302:XTW:CAK	2.31	0.61
1:E:207:LEU:C	1:E:211:ALA:HB2	2.21	0.60
1:E:207:LEU:HB2	1:E:211:ALA:HA	1.84	0.59
1:G:216:GLN:N	1:G:216:GLN:OE1	2.34	0.59
4:A:424:HOH:O	1:G:2:THR:HG21	2.02	0.58
1:A:43:ARG:HB3	1:A:46:LEU:HD13	1.86	0.57
1:A:46:LEU:H	1:A:46:LEU:HD12	1.72	0.55
1:E:43:ARG:HB3	1:E:46:LEU:HD13	1.91	0.53
1:A:218:LEU:HD23	3:A:302:XTW:CAK	2.39	0.51
1:E:207:LEU:HB2	1:E:211:ALA:CA	2.40	0.51
1:E:236:THR:HB	1:E:237:PRO:HD3	1.91	0.51
1:A:202:ILE:O	1:A:206:ALA:HB2	2.12	0.50
2:A:301:NAD:C7N	3:A:302:XTW:CAG	2.89	0.50
1:B:218:LEU:HD23	3:B:302:XTW:CAK	2.41	0.50
1:A:236:THR:HB	1:A:237:PRO:HD3	1.93	0.50
1:G:220:GLU:O	1:G:224:GLN:HB2	2.11	0.49
1:A:220:GLU:O	1:A:224:GLN:HB2	2.13	0.49
1:A:207:LEU:HB2	1:A:211:ALA:HB1	1.95	0.48
1:E:220:GLU:O	1:E:224:GLN:HB2	2.14	0.47
1:G:150:ASP:OD1	1:G:152:SER:HB3	2.14	0.47
1:B:220:GLU:O	1:B:224:GLN:HB2	2.13	0.47
1:A:46:LEU:N	1:A:46:LEU:HD12	2.29	0.47
1:A:208:GLY:C	1:A:211:ALA:CB	2.84	0.47
1:E:202:ILE:O	1:E:206:ALA:HB2	2.14	0.47
1:E:208:GLY:C	1:E:211:ALA:CB	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:THR:HG22	4:A:434:HOH:O	2.15	0.46
1:A:213:ALA:O	1:A:216:GLN:HB2	2.16	0.46
1:A:150:ASP:OD1	1:A:152:SER:OG	2.33	0.45
1:B:2:THR:HA	1:E:2:THR:CB	2.47	0.44
1:B:156:PRO:HD3	1:G:269:LEU:C	2.38	0.44
1:A:207:LEU:HB3	1:A:211:ALA:HA	1.99	0.44
1:B:236:THR:HB	1:B:237:PRO:HD3	1.99	0.44
1:A:225:ARG:NH1	1:A:268:LEU:O	2.51	0.43
1:A:219:GLU:OE1	3:A:302:XTW:NAN	2.51	0.43
1:E:203:VAL:O	1:E:207:LEU:HD12	2.19	0.43
1:G:113:TYR:CE2	1:G:117:SER:HB2	2.54	0.43
1:A:209:GLU:N	1:A:211:ALA:HB2	2.34	0.42
1:E:113:TYR:CE2	1:E:117:SER:HB2	2.54	0.42
1:A:113:TYR:CE2	1:A:117:SER:HB2	2.54	0.42
1:E:148:ASP:OD2	1:E:169:GLU:OE2	2.37	0.42
1:B:153:ARG:NH2	1:G:153:ARG:NE	2.66	0.42
1:B:48:GLN:HG3	4:B:414:HOH:O	2.19	0.42
1:E:193:PRO:HA	2:E:301:NAD:O7N	2.19	0.42
1:A:148:ASP:OD2	1:A:169:GLU:OE2	2.38	0.41
1:B:41:PHE:HB2	2:B:301:NAD:C2A	2.50	0.41
1:B:148:ASP:OD2	1:B:169:GLU:OE2	2.37	0.41
1:G:148:ASP:OD2	1:G:169:GLU:OE2	2.39	0.41
1:A:203:VAL:O	1:A:207:LEU:HD12	2.20	0.41
1:E:46:LEU:N	1:E:46:LEU:HD12	2.30	0.41
1:B:113:TYR:CE2	1:B:117:SER:HB2	2.55	0.40
1:G:67:ASN:O	1:G:68:GLU:C	2.59	0.40
1:B:269:LEU:HD12	1:B:269:LEU:HA	1.83	0.40
1:A:67:ASN:O	1:A:68:GLU:C	2.59	0.40
1:B:67:ASN:O	1:B:68:GLU:C	2.60	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	266/289 (92%)	241 (91%)	22 (8%)	3 (1%)	17	36
1	B	257/289 (89%)	238 (93%)	15 (6%)	4 (2%)	12	24
1	E	268/289 (93%)	244 (91%)	20 (8%)	4 (2%)	13	26
1	G	261/289 (90%)	240 (92%)	16 (6%)	5 (2%)	10	19
All	All	1052/1156 (91%)	963 (92%)	73 (7%)	16 (2%)	13	26

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	211	ALA
1	A	212	GLY
1	B	212	GLY
1	E	212	GLY
1	G	212	GLY
1	B	195	ARG
1	G	215	ILE
1	G	221	GLY
1	A	195	ARG
1	E	221	GLY
1	G	195	ARG
1	B	221	GLY
1	G	210	GLU
1	A	221	GLY
1	E	215	ILE
1	B	215	ILE

### 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	204/222 (92%)	187 (92%)	17 (8%)	14	27
1	B	201/222 (90%)	189 (94%)	12 (6%)	24	47
1	E	206/222 (93%)	191 (93%)	15 (7%)	17	35
1	G	204/222 (92%)	194 (95%)	10 (5%)	31	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	815/888 (92%)	761 (93%)	54 (7%)	20	40

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

Mol	Chain	Res	Type
1	A	17	THR
1	A	39	THR
1	A	45	ARG
1	A	46	LEU
1	A	49	ARG
1	A	67	ASN
1	A	69	GLU
1	A	79	THR
1	A	152	SER
1	A	170	SER
1	A	202	ILE
1	A	207	LEU
1	A	215	ILE
1	A	216	GLN
1	A	217	LEU
1	A	224	GLN
1	A	269	LEU
1	B	17	THR
1	B	39	THR
1	B	43	ARG
1	B	79	THR
1	B	105	ILE
1	B	132	LYS
1	B	170	SER
1	B	200	SER
1	B	203	VAL
1	B	216	GLN
1	B	220	GLU
1	B	224	GLN
1	E	17	THR
1	E	45	ARG
1	E	79	THR
1	E	152	SER
1	E	170	SER
1	E	195	ARG
1	E	200	SER
1	E	202	ILE

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Mol	Chain	Res	Type
1	E	207	LEU
1	E	214	GLN
1	E	220	GLU
1	E	224	GLN
1	E	237	PRO
1	E	258	ILE
1	E	269	LEU
1	G	17	THR
1	G	39	THR
1	G	79	THR
1	G	105	ILE
1	G	170	SER
1	G	203	VAL
1	G	210	GLU
1	G	214	GLN
1	G	224	GLN
1	G	269	LEU

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

Mol	Chain	Res	Type
1	A	67	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

8 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	NAD	A	301	-	42,48,48	0.96	2 (4%)	46,73,73	1.40	7 (15%)
3	XTW	A	302	-	26,27,27	2.18	7 (26%)	36,38,38	2.37	7 (19%)
2	NAD	B	301	-	42,48,48	0.74	1 (2%)	46,73,73	1.33	4 (8%)
3	XTW	B	302	-	26,27,27	3.76	6 (23%)	36,38,38	2.42	9 (25%)
2	NAD	E	301	-	42,48,48	0.67	0	46,73,73	1.51	7 (15%)
3	XTW	E	302	-	26,27,27	2.77	8 (30%)	36,38,38	1.69	7 (19%)
2	NAD	G	301	-	42,48,48	0.78	1 (2%)	46,73,73	1.03	2 (4%)
3	XTW	G	302	-	26,27,27	3.52	5 (19%)	36,38,38	2.39	6 (16%)

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	NAD	A	301	-	-	0/22/62/62	0/5/5/5
3	XTW	A	302	-	-	0/12/14/14	0/3/4/4
2	NAD	B	301	-	-	0/22/62/62	0/5/5/5
3	XTW	B	302	-	-	0/12/14/14	0/3/4/4
2	NAD	E	301	-	-	0/22/62/62	0/5/5/5
3	XTW	E	302	-	-	1/12/14/14	0/3/4/4
2	NAD	G	301	-	-	0/22/62/62	0/5/5/5
3	XTW	G	302	-	-	0/12/14/14	0/3/4/4

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	302	XTW	NAN-NAO	-13.39	1.15	1.34
3	B	302	XTW	NAO-NAX	-13.16	1.08	1.34
3	B	302	XTW	NAN-NAO	-11.22	1.18	1.34
3	E	302	XTW	NAN-NAO	-10.15	1.19	1.34
3	G	302	XTW	NAO-NAX	-9.89	1.15	1.34
3	A	302	XTW	NAO-NAX	-5.91	1.23	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	XTW	CAM-CAR	-5.83	1.37	1.51
3	A	302	XTW	CAM-CAR	-5.48	1.38	1.51
3	E	302	XTW	NAO-NAX	-5.39	1.24	1.34
3	E	302	XTW	CAM-CAR	-5.05	1.39	1.51
3	G	302	XTW	CAM-CAR	-4.63	1.40	1.51
3	A	302	XTW	NAN-NAO	-4.04	1.28	1.34
3	B	302	XTW	CAT-NAN	-3.24	1.30	1.34
3	B	302	XTW	CAS-CL	-3.14	1.65	1.73
2	B	301	NAD	O4D-C1D	-2.92	1.37	1.41
3	E	302	XTW	CAS-CL	-2.87	1.66	1.73
3	G	302	XTW	CAT-NAN	-2.76	1.30	1.34
2	G	301	NAD	O4D-C1D	-2.69	1.37	1.41
3	G	302	XTW	CAJ-NAX	-2.69	1.32	1.35
3	E	302	XTW	OAP-CAV	-2.35	1.34	1.39
3	B	302	XTW	CAJ-NAX	-2.32	1.32	1.35
3	A	302	XTW	OAP-CAU	-2.27	1.34	1.39
3	E	302	XTW	CAJ-NAX	-2.15	1.33	1.35
3	A	302	XTW	CAT-NAN	-2.05	1.31	1.34
3	E	302	XTW	CAT-NAN	-2.04	1.31	1.34
2	A	301	NAD	C3N-C7N	2.36	1.54	1.50
3	A	302	XTW	CAM-NAX	2.82	1.52	1.47
3	E	302	XTW	CAM-NAX	3.10	1.52	1.47
3	A	302	XTW	CAS-CL	3.69	1.83	1.73
2	A	301	NAD	C2N-N1N	4.31	1.41	1.35

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	XTW	CAK-CAW-CAT	-10.40	110.02	120.12
3	G	302	XTW	CAK-CAW-CAT	-6.77	113.55	120.12
2	A	301	NAD	C4B-O4B-C1B	-6.16	103.11	109.64
2	B	301	NAD	C4B-O4B-C1B	-5.85	103.44	109.64
3	B	302	XTW	CAM-NAX-CAJ	-4.72	123.17	129.19
2	E	301	NAD	O4D-C1D-N1N	-4.46	103.29	108.10
2	E	301	NAD	C4B-O4B-C1B	-4.35	105.03	109.64
3	B	302	XTW	CAK-CAW-CAT	-4.22	116.03	120.12
2	G	301	NAD	C4B-O4B-C1B	-3.83	105.58	109.64
3	E	302	XTW	CAK-CAW-CAT	-3.74	116.48	120.12
3	A	302	XTW	CAR-CAM-NAX	-3.69	106.74	112.17
3	A	302	XTW	OAP-CAV-CAS	-3.27	112.21	119.83
3	B	302	XTW	CAL-CAW-CAT	-3.26	116.95	120.12
3	G	302	XTW	CAR-CAM-NAX	-3.17	107.50	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	NAD	C1B-N9A-C4A	-3.12	123.33	126.81
2	E	301	NAD	O2A-PA-O3	-3.06	92.14	105.27
2	E	301	NAD	C1B-N9A-C4A	-2.96	123.50	126.81
3	E	302	XTW	CAR-CAM-NAX	-2.91	107.89	112.17
2	A	301	NAD	O4D-C1D-N1N	-2.63	105.26	108.10
2	B	301	NAD	C1B-N9A-C4A	-2.54	123.97	126.81
3	G	302	XTW	CAT-CAJ-NAX	-2.52	102.80	106.97
2	A	301	NAD	O2A-PA-O3	-2.51	94.49	105.27
2	B	301	NAD	O2D-C2D-C1D	-2.51	103.76	111.61
3	B	302	XTW	CAL-CAK-CAW	-2.46	59.21	60.63
3	E	302	XTW	CAL-CAW-CAT	-2.43	117.76	120.12
2	G	301	NAD	O2A-PA-O3	-2.40	94.98	105.27
3	B	302	XTW	CAT-CAJ-NAX	-2.38	103.04	106.97
3	E	302	XTW	OAP-CAV-CAS	-2.07	115.00	119.83
2	E	301	NAD	O2N-PN-O5D	2.02	117.84	108.24
3	B	302	XTW	CAK-CAW-CAL	2.16	60.50	58.73
2	A	301	NAD	O5D-C5D-C4D	2.17	116.91	109.09
3	A	302	XTW	CAF-CAV-CAS	2.23	122.59	118.79
2	E	301	NAD	O2A-PA-O1A	2.24	124.19	112.56
2	A	301	NAD	O2A-PA-O1A	2.28	124.41	112.56
2	B	301	NAD	O4D-C1D-N1N	2.34	110.63	108.10
2	A	301	NAD	C2D-C1D-N1N	2.50	118.44	113.53
3	E	302	XTW	CAW-CAT-NAN	2.66	124.72	120.09
3	G	302	XTW	CAW-CAT-NAN	2.71	124.82	120.09
3	E	302	XTW	CAV-CAS-CL	2.93	123.02	119.40
3	A	302	XTW	NAN-NAO-NAX	3.00	109.58	107.31
2	E	301	NAD	C2D-C1D-N1N	3.31	120.02	113.53
3	G	302	XTW	CAV-CAS-CL	3.35	123.53	119.40
3	A	302	XTW	CAU-OAP-CAV	3.35	126.21	117.84
3	A	302	XTW	CAL-CAW-CAT	3.41	123.43	120.12
3	B	302	XTW	CAV-CAS-CL	3.57	123.81	119.40
3	B	302	XTW	CAW-CAT-NAN	4.33	127.62	120.09
3	E	302	XTW	NAN-NAO-NAX	5.47	111.44	107.31
3	B	302	XTW	NAN-NAO-NAX	9.36	114.37	107.31
3	G	302	XTW	NAN-NAO-NAX	10.36	115.12	107.31

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	302	XTW	CAK-CAW-CAT-CAJ

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NAD	1	0
3	A	302	XTW	3	0
2	B	301	NAD	1	0
3	B	302	XTW	1	0
2	E	301	NAD	1	0
3	G	302	XTW	1	0

## 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	268/289 (92%)	0.04	11 (4%) 41 33	44, 75, 115, 137	0
1	B	261/289 (90%)	0.07	14 (5%) 29 22	46, 79, 114, 127	0
1	E	268/289 (92%)	-0.37	3 (1%) 82 79	34, 55, 93, 120	0
1	G	264/289 (91%)	0.33	23 (8%) 13 8	44, 80, 121, 132	0
All	All	1061/1156 (91%)	0.01	51 (4%) 34 27	34, 73, 117, 137	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	60	LEU	5.0
1	A	207	LEU	4.6
1	B	211	ALA	4.6
1	B	216	GLN	4.4
1	B	217	LEU	4.4
1	B	218	LEU	4.3
1	G	218	LEU	4.3
1	B	212	GLY	4.2
1	B	84	ALA	3.9
1	G	59	PRO	3.9
1	G	47	ILE	3.8
1	G	57	LYS	3.7
1	B	215	ILE	3.7
1	G	81	ALA	3.6
1	A	201	ALA	3.5
1	B	213	ALA	3.5
1	A	209	GLU	3.5
1	G	45	ARG	3.4
1	G	210	GLU	3.4
1	G	54	LEU	3.3
1	A	2	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	44	LEU	3.3
1	E	204	GLY	3.2
1	G	63	LEU	3.2
1	G	2	THR	2.8
1	G	56	ALA	2.8
1	G	61	LEU	2.8
1	A	84	ALA	2.8
1	B	269	LEU	2.8
1	B	214	GLN	2.7
1	G	82	ILE	2.7
1	G	80	GLU	2.6
1	E	215	ILE	2.6
1	E	207	LEU	2.6
1	G	52	ASP	2.6
1	B	76	GLY	2.6
1	A	202	ILE	2.5
1	B	105	ILE	2.5
1	G	58	ALA	2.5
1	A	45	ARG	2.5
1	B	81	ALA	2.5
1	G	9	ARG	2.4
1	A	78	VAL	2.3
1	A	57	LYS	2.3
1	A	205	GLY	2.2
1	G	35	GLN	2.2
1	G	62	GLU	2.2
1	A	208	GLY	2.2
1	G	214	GLN	2.1
1	G	217	LEU	2.1
1	B	86	ASN	2.0

## 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 [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. 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
3	XTW	G	302	24/24	0.95	0.16	-0.23	48,70,77,79	0
3	XTW	E	302	24/24	0.98	0.14	-0.27	41,57,62,67	0
3	XTW	B	302	24/24	0.96	0.16	-0.36	53,62,70,84	0
3	XTW	A	302	24/24	0.95	0.13	-0.48	48,57,70,72	0
2	NAD	A	301	44/44	0.95	0.13	-0.52	44,60,71,83	0
2	NAD	E	301	44/44	0.97	0.10	-0.71	31,38,52,55	0
2	NAD	B	301	44/44	0.95	0.13	-0.80	49,70,81,93	0
2	NAD	G	301	44/44	0.96	0.12	-0.95	49,71,82,89	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.