



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 15, 2018 – 07:48 PM EST

PDB ID : 3ZX0  
Title : NTPDase1 in complex with Heptamolybdate  
Authors : Zebisch, M.; Schaefer, P.; Straeter, N.  
Deposited on : 2011-08-04  
Resolution : 2.50 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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-20030736

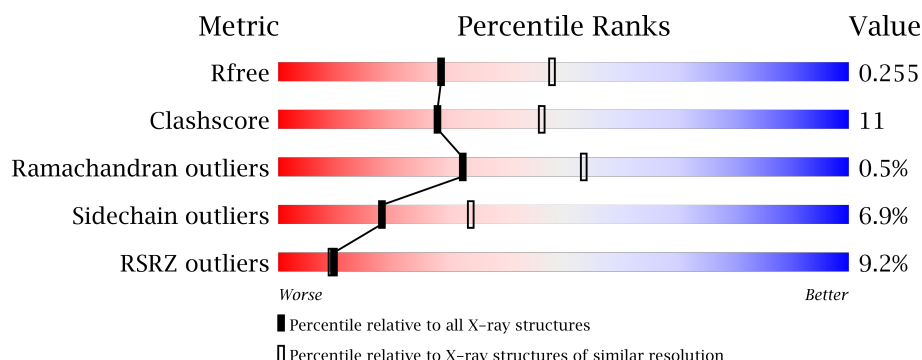
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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	452	<div> <div>10%</div> <div>63% 19% 15%</div> </div>
1	B	452	<div> <div>11%</div> <div>64% 20% 15%</div> </div>
1	C	452	<div> <div>8%</div> <div>64% 20% 13%</div> </div>
1	D	452	<div> <div>4%</div> <div>68% 19% 12%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACY	A	511	-	-	X	-
3	ACY	B	511	-	-	-	X
3	ACY	B	512	-	-	-	X
3	ACY	C	511	-	-	X	-
3	ACY	C	512	-	-	-	X
4	MO7	B	531[A]	-	-	X	-
4	MO7	C	531[B]	-	-	X	-
4	MO7	D	531	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12434 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 ECTONUCLEOSIDE TRIPHOSPHATE DIPHOSPHOHYDROLASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	2	0
			3026	1958	486	562	20			
1	B	386	Total	C	N	O	S	0	1	0
			2994	1935	482	558	19			
1	C	393	Total	C	N	O	S	0	2	0
			3115	2020	499	576	20			
1	D	397	Total	C	N	O	S	0	3	0
			3121	2021	504	576	20			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	MET	-	expression tag	UNP P97687
A	16	ALA	-	expression tag	UNP P97687
A	17	HIS	-	expression tag	UNP P97687
A	18	HIS	-	expression tag	UNP P97687
A	19	HIS	-	expression tag	UNP P97687
A	20	HIS	-	expression tag	UNP P97687
A	21	HIS	-	expression tag	UNP P97687
A	22	HIS	-	expression tag	UNP P97687
A	23	VAL	-	expression tag	UNP P97687
A	24	GLY	-	expression tag	UNP P97687
A	25	THR	-	expression tag	UNP P97687
A	26	GLY	-	expression tag	UNP P97687
A	27	SER	-	expression tag	UNP P97687
A	28	ASN	-	expression tag	UNP P97687
A	29	ASP	-	expression tag	UNP P97687
A	30	ASP	-	expression tag	UNP P97687
A	31	ASP	-	expression tag	UNP P97687
A	32	ASP	-	expression tag	UNP P97687
A	33	LYS	-	expression tag	UNP P97687
A	34	SER	-	expression tag	UNP P97687

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	PRO	-	expression tag	UNP P97687
A	36	ASP	-	expression tag	UNP P97687
A	37	PRO	-	expression tag	UNP P97687
A	80	GLN	LEU	SEE REMARK 999	UNP P97687
A	190	LYS	-	linker	UNP P97687
A	191	THR	-	linker	UNP P97687
A	192	PRO	-	linker	UNP P97687
A	204	GLY	-	linker	UNP P97687
A	205	GLY	-	linker	UNP P97687
A	206	SER	-	linker	UNP P97687
A	220	ILE	VAL	SEE REMARK 999	UNP P97687
A	227	SER	GLN	SEE REMARK 999	UNP P97687
A	331	ILE	PHE	conflict	UNP P97687
B	15	MET	-	expression tag	UNP P97687
B	16	ALA	-	expression tag	UNP P97687
B	17	HIS	-	expression tag	UNP P97687
B	18	HIS	-	expression tag	UNP P97687
B	19	HIS	-	expression tag	UNP P97687
B	20	HIS	-	expression tag	UNP P97687
B	21	HIS	-	expression tag	UNP P97687
B	22	HIS	-	expression tag	UNP P97687
B	23	VAL	-	expression tag	UNP P97687
B	24	GLY	-	expression tag	UNP P97687
B	25	THR	-	expression tag	UNP P97687
B	26	GLY	-	expression tag	UNP P97687
B	27	SER	-	expression tag	UNP P97687
B	28	ASN	-	expression tag	UNP P97687
B	29	ASP	-	expression tag	UNP P97687
B	30	ASP	-	expression tag	UNP P97687
B	31	ASP	-	expression tag	UNP P97687
B	32	ASP	-	expression tag	UNP P97687
B	33	LYS	-	expression tag	UNP P97687
B	34	SER	-	expression tag	UNP P97687
B	35	PRO	-	expression tag	UNP P97687
B	36	ASP	-	expression tag	UNP P97687
B	37	PRO	-	expression tag	UNP P97687
B	80	GLN	LEU	SEE REMARK 999	UNP P97687
B	190	LYS	-	linker	UNP P97687
B	191	THR	-	linker	UNP P97687
B	192	PRO	-	linker	UNP P97687
B	204	GLY	-	linker	UNP P97687
B	205	GLY	-	linker	UNP P97687

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	206	SER	-	linker	UNP P97687
B	220	ILE	VAL	SEE REMARK 999	UNP P97687
B	227	SER	GLN	SEE REMARK 999	UNP P97687
B	331	ILE	PHE	conflict	UNP P97687
C	15	MET	-	expression tag	UNP P97687
C	16	ALA	-	expression tag	UNP P97687
C	17	HIS	-	expression tag	UNP P97687
C	18	HIS	-	expression tag	UNP P97687
C	19	HIS	-	expression tag	UNP P97687
C	20	HIS	-	expression tag	UNP P97687
C	21	HIS	-	expression tag	UNP P97687
C	22	HIS	-	expression tag	UNP P97687
C	23	VAL	-	expression tag	UNP P97687
C	24	GLY	-	expression tag	UNP P97687
C	25	THR	-	expression tag	UNP P97687
C	26	GLY	-	expression tag	UNP P97687
C	27	SER	-	expression tag	UNP P97687
C	28	ASN	-	expression tag	UNP P97687
C	29	ASP	-	expression tag	UNP P97687
C	30	ASP	-	expression tag	UNP P97687
C	31	ASP	-	expression tag	UNP P97687
C	32	ASP	-	expression tag	UNP P97687
C	33	LYS	-	expression tag	UNP P97687
C	34	SER	-	expression tag	UNP P97687
C	35	PRO	-	expression tag	UNP P97687
C	36	ASP	-	expression tag	UNP P97687
C	37	PRO	-	expression tag	UNP P97687
C	80	GLN	LEU	SEE REMARK 999	UNP P97687
C	190	LYS	-	linker	UNP P97687
C	191	THR	-	linker	UNP P97687
C	192	PRO	-	linker	UNP P97687
C	204	GLY	-	linker	UNP P97687
C	205	GLY	-	linker	UNP P97687
C	206	SER	-	linker	UNP P97687
C	220	ILE	VAL	SEE REMARK 999	UNP P97687
C	227	SER	GLN	SEE REMARK 999	UNP P97687
C	331	ILE	PHE	conflict	UNP P97687
D	15	MET	-	expression tag	UNP P97687
D	16	ALA	-	expression tag	UNP P97687
D	17	HIS	-	expression tag	UNP P97687
D	18	HIS	-	expression tag	UNP P97687
D	19	HIS	-	expression tag	UNP P97687

*Continued on next page...*

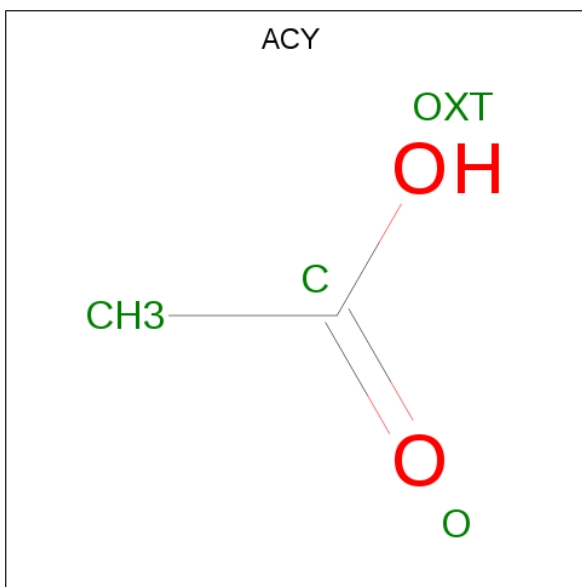
*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	20	HIS	-	expression tag	UNP P97687
D	21	HIS	-	expression tag	UNP P97687
D	22	HIS	-	expression tag	UNP P97687
D	23	VAL	-	expression tag	UNP P97687
D	24	GLY	-	expression tag	UNP P97687
D	25	THR	-	expression tag	UNP P97687
D	26	GLY	-	expression tag	UNP P97687
D	27	SER	-	expression tag	UNP P97687
D	28	ASN	-	expression tag	UNP P97687
D	29	ASP	-	expression tag	UNP P97687
D	30	ASP	-	expression tag	UNP P97687
D	31	ASP	-	expression tag	UNP P97687
D	32	ASP	-	expression tag	UNP P97687
D	33	LYS	-	expression tag	UNP P97687
D	34	SER	-	expression tag	UNP P97687
D	35	PRO	-	expression tag	UNP P97687
D	36	ASP	-	expression tag	UNP P97687
D	37	PRO	-	expression tag	UNP P97687
D	80	GLN	LEU	SEE REMARK 999	UNP P97687
D	190	LYS	-	linker	UNP P97687
D	191	THR	-	linker	UNP P97687
D	192	PRO	-	linker	UNP P97687
D	204	GLY	-	linker	UNP P97687
D	205	GLY	-	linker	UNP P97687
D	206	SER	-	linker	UNP P97687
D	220	ILE	VAL	SEE REMARK 999	UNP P97687
D	227	SER	GLN	SEE REMARK 999	UNP P97687
D	331	ILE	PHE	conflict	UNP P97687

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	5	Total Cl 5 5	0	0
2	A	4	Total Cl 4 4	0	0
2	D	8	Total Cl 8 8	0	0
2	C	5	Total Cl 5 5	0	0

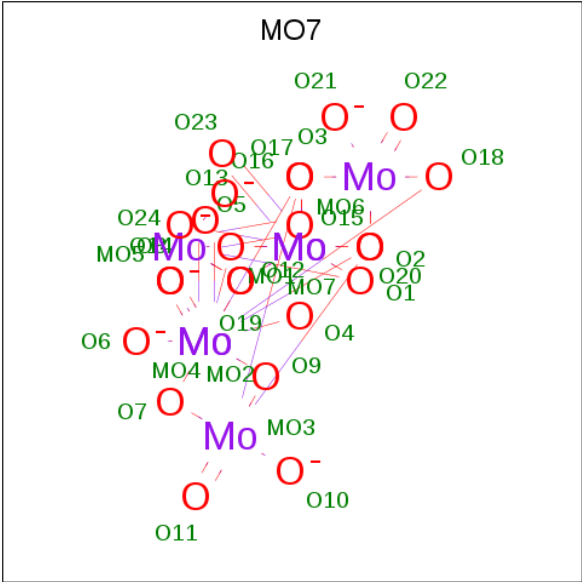
- Molecule 3 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



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

- Molecule 4 is bis(mu4-oxo)-bis(mu3-oxo)-octakis(mu2-oxo)-dodecaoxo-heptamolybdenum (VI) (three-letter code: MO7) (formula: Mo<sub>7</sub>O<sub>24</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Mo	O	0	0
			31	7	24		
4	B	1	Total	Mo	O	0	1
			31	7	24		
4	C	1	Total	Mo	O	0	1
			31	7	24		
4	D	1	Total	Mo	O	0	0
			31	7	24		

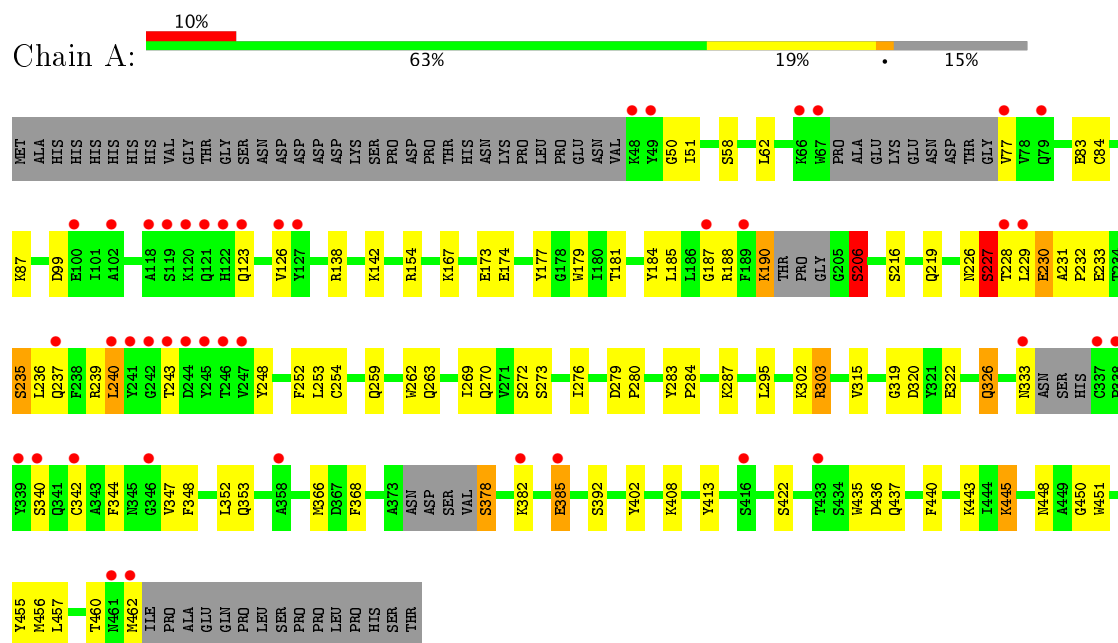
- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Na	0	0
			1	1		
5	D	1	Total	Na	0	0
			1	1		
5	C	2	Total	Na	0	0
			2	2		

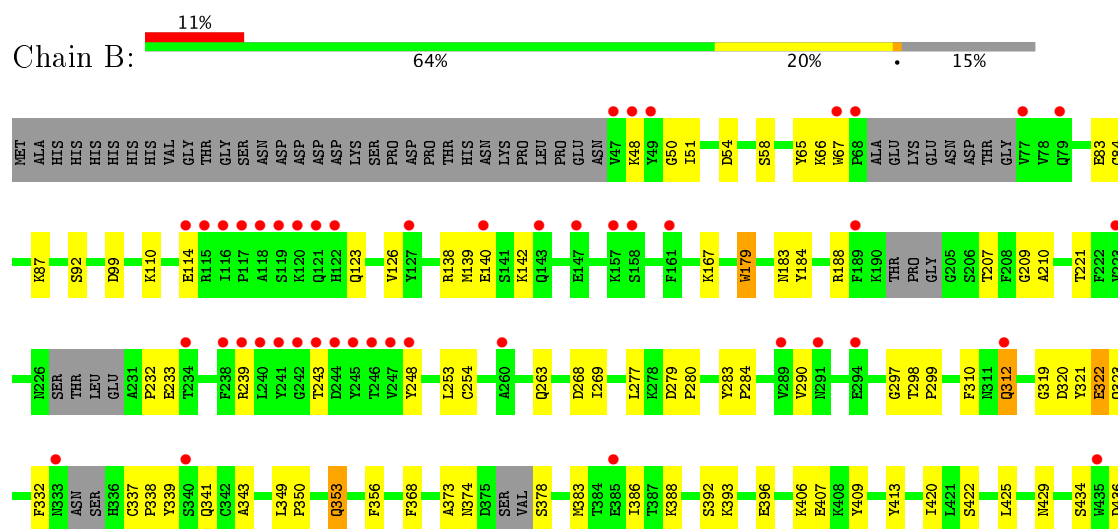
### 3 Residue-property plots

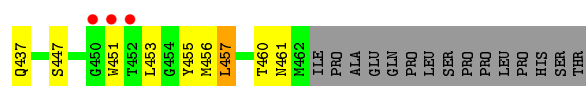
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: ECTONUCLEOSIDE TRIPHOSPHATE DIPHOSPHOHYDROLASE 1

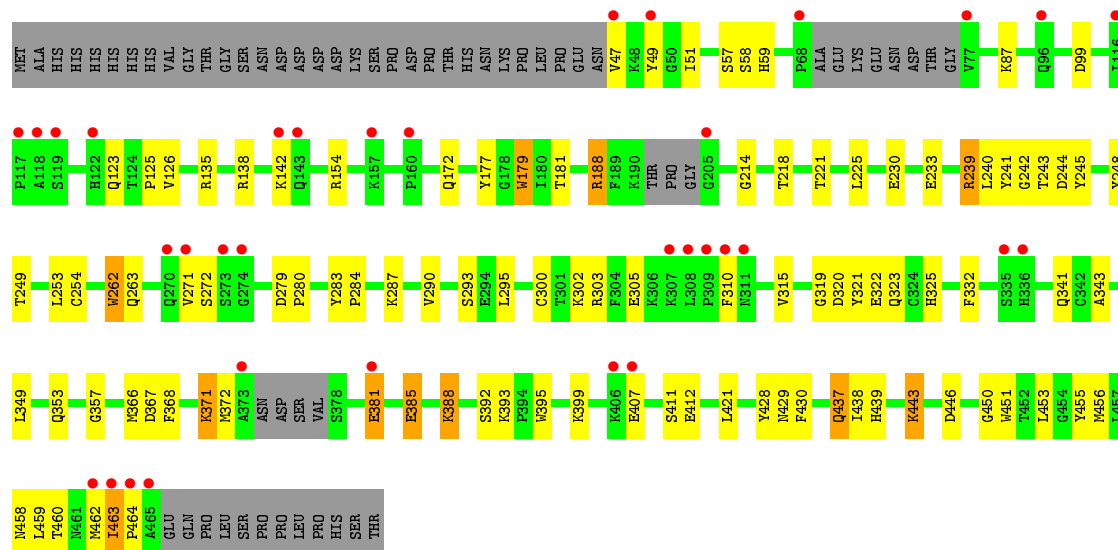


#### • Molecule 1: ECTONUCLEOSIDE TRIPHOSPHATE DIPHOSPHOHYDROLASE 1

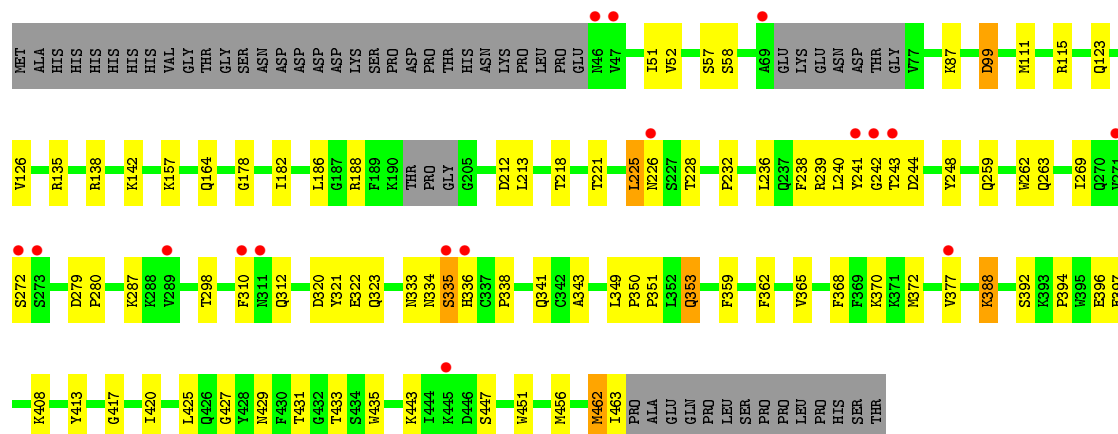




• Molecule 1: ECTONUCLEOSIDE TRIPHOSPHATE DIPHOSPHOHYDROLASE 1



• Molecule 1: ECTONUCLEOSIDE TRIPHOSPHATE DIPHOSPHOHYDROLASE 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	163.81Å 80.27Å 164.92Å 90.00° 117.92° 90.00°	Depositor
Resolution (Å)	145.73 – 2.50 28.75 – 2.50	Depositor EDS
% Data completeness (in resolution range)	87.6 (145.73-2.50) 88.0 (28.75-2.50)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.213 , 0.257 0.213 , 0.255	Depositor DCC
$R_{free}$ test set	1157 reflections (2.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.4	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 43.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.007 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12434	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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: NA, ACY, MO7, CL

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	0.82	4/3110 (0.1%)	0.93	4/4203 (0.1%)
1	B	0.79	3/3073 (0.1%)	0.85	4/4158 (0.1%)
1	C	0.90	4/3204 (0.1%)	0.98	6/4334 (0.1%)
1	D	0.93	6/3213 (0.2%)	1.03	10/4351 (0.2%)
All	All	0.86	17/12600 (0.1%)	0.95	24/17046 (0.1%)

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	1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	135	ARG	CZ-NH1	-8.23	1.22	1.33
1	D	135	ARG	CZ-NH2	-6.76	1.24	1.33
1	D	451	TRP	CD2-CE2	6.37	1.49	1.41
1	C	179	TRP	CD2-CE2	6.08	1.48	1.41
1	A	451	TRP	CD2-CE2	5.77	1.48	1.41
1	B	451	TRP	CD2-CE2	5.77	1.48	1.41
1	A	435	TRP	CD2-CE2	5.53	1.48	1.41
1	B	67	TRP	CD2-CE2	5.52	1.48	1.41
1	B	179	TRP	CD2-CE2	5.33	1.47	1.41
1	D	262[A]	TRP	CD2-CE2	5.29	1.47	1.41
1	D	262[B]	TRP	CD2-CE2	5.29	1.47	1.41
1	A	179	TRP	CD2-CE2	5.28	1.47	1.41
1	C	262[A]	TRP	CD2-CE2	5.27	1.47	1.41
1	C	262[B]	TRP	CD2-CE2	5.27	1.47	1.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	385	GLU	CG-CD	5.22	1.59	1.51
1	D	435	TRP	CD2-CE2	5.11	1.47	1.41
1	C	451	TRP	CD2-CE2	5.05	1.47	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	138	ARG	NE-CZ-NH1	13.29	126.94	120.30
1	A	138	ARG	NE-CZ-NH2	-12.99	113.81	120.30
1	C	138	ARG	NE-CZ-NH1	12.14	126.37	120.30
1	D	138	ARG	NE-CZ-NH2	-11.77	114.42	120.30
1	D	135	ARG	NE-CZ-NH1	11.31	125.96	120.30
1	A	138	ARG	NE-CZ-NH1	10.97	125.78	120.30
1	C	138	ARG	NE-CZ-NH2	-10.58	115.01	120.30
1	D	135	ARG	NE-CZ-NH2	10.52	125.56	120.30
1	D	135	ARG	NH1-CZ-NH2	-10.00	108.40	119.40
1	B	138	ARG	NE-CZ-NH1	8.47	124.54	120.30
1	B	138	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	D	138	ARG	CD-NE-CZ	6.82	133.15	123.60
1	D	212	ASP	CB-CG-OD2	-6.53	112.43	118.30
1	C	135	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	D	236	LEU	CA-CB-CG	6.06	129.24	115.30
1	B	268	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	138	ARG	CD-NE-CZ	5.77	131.68	123.60
1	C	230	GLU	OE1-CD-OE2	-5.62	116.56	123.30
1	C	450	GLY	N-CA-C	-5.50	99.34	113.10
1	A	276	ILE	CB-CA-C	-5.50	100.60	111.60
1	B	54	ASP	CB-CG-OD1	5.47	123.23	118.30
1	C	412	GLU	CB-CA-C	-5.31	99.78	110.40
1	D	287	LYS	CA-CB-CG	5.30	125.06	113.40
1	D	372	MET	CB-CG-SD	-5.05	97.25	112.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	206	SER	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	3026	0	2900	78	0
1	B	2994	0	2847	74	0
1	C	3115	0	3024	59	0
1	D	3121	0	3007	46	0
2	A	4	0	0	1	0
2	B	5	0	0	2	0
2	C	5	0	0	3	0
2	D	8	0	0	3	0
3	A	4	0	3	3	0
3	B	8	0	6	1	0
3	C	8	0	6	4	0
3	D	8	0	6	2	0
4	A	31	0	0	6	0
4	B	31	0	0	8	0
4	C	31	0	0	13	0
4	D	31	0	0	7	0
5	B	1	0	0	0	0
5	C	2	0	0	0	0
5	D	1	0	0	0	0
All	All	12434	0	11799	272	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 11.

All (272) 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:230:GLU:C	1:A:232:PRO:HD3	1.53	1.29
1:D:225:LEU:HD13	1:D:353:GLN:NE2	1.56	1.20
1:A:167:LYS:HD2	1:B:232:PRO:HG2	1.15	1.14
1:D:225:LEU:HD13	1:D:353:GLN:HE21	0.98	1.12
1:A:231:ALA:N	1:A:232:PRO:HD3	1.71	1.04
1:A:366:MET:HE2	3:A:511:ACY:H1	1.45	0.97
1:A:50:GLY:HA3	1:A:456:MET:CE	1.93	0.97
1:A:167:LYS:CD	1:B:232:PRO:HG2	1.94	0.95

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:531[B]:MO7:O17	4:C:531[B]:MO7:O21	1.86	0.92
1:C:225:LEU:HG	1:C:353:GLN:NE2	1.86	0.91
1:A:167:LYS:HD2	1:B:232:PRO:CG	2.04	0.87
1:D:225:LEU:CD1	1:D:353:GLN:NE2	2.39	0.85
1:B:50:GLY:HA3	1:B:456:MET:HE3	1.57	0.85
1:A:226:ASN:O	1:A:227:SER:OG	1.95	0.84
1:C:262[B]:TRP:HE3	1:C:295:LEU:HD12	1.44	0.82
1:A:366:MET:CE	3:A:511:ACY:H1	2.09	0.82
1:B:322:GLU:HA	1:B:322:GLU:OE1	1.79	0.80
1:C:407:GLU:O	1:C:411:SER:HB2	1.82	0.80
1:B:407:GLU:HG3	4:C:531[B]:MO7:O18	1.82	0.79
4:C:531[B]:MO7:O18	4:C:531[B]:MO7:O21	2.01	0.79
1:A:230:GLU:C	1:A:232:PRO:CD	2.45	0.78
4:B:531[A]:MO7:O22	4:B:531[A]:MO7:O6	2.02	0.78
4:D:531:MO7:O21	4:D:531:MO7:O23	2.01	0.77
1:D:52:VAL:HG23	1:D:456:MET:HE3	1.69	0.74
1:A:231:ALA:N	1:A:232:PRO:CD	2.49	0.74
1:C:233:GLU:HG2	2:C:506:CL:CL	2.26	0.73
1:B:50:GLY:HA3	1:B:456:MET:CE	2.19	0.72
1:C:279:ASP:OD1	1:C:280:PRO:HD2	1.89	0.72
1:C:188:ARG:HH11	1:C:188:ARG:CG	2.03	0.71
1:D:239:ARG:HE	1:D:242:GLY:HA2	1.55	0.71
1:A:50:GLY:HA3	1:A:456:MET:HE3	1.72	0.71
1:B:140:GLU:OE2	1:B:297:GLY:O	2.09	0.70
1:B:406:LYS:HG2	4:B:531[A]:MO7:O4	1.92	0.70
1:B:434:SER:O	1:B:437:GLN:HG2	1.93	0.68
1:A:177:TYR:CE1	1:A:455:TYR:HA	2.30	0.67
4:C:531[B]:MO7:O24	4:C:531[B]:MO7:O22	2.13	0.67
1:B:290:VAL:O	1:B:312:GLN:HB2	1.95	0.67
1:B:368:PHE:CG	1:B:413:TYR:CE2	2.83	0.67
1:C:366:MET:CE	3:C:511:ACY:H1	2.25	0.66
1:B:368:PHE:CB	1:B:413:TYR:HE2	2.09	0.66
1:C:172:GLN:HG2	1:C:249:THR:HG23	1.78	0.65
1:C:262[B]:TRP:CE3	1:C:295:LEU:HD12	2.29	0.65
1:D:462:MET:O	1:D:463:ILE:CB	2.44	0.65
1:D:239:ARG:NE	1:D:242:GLY:HA2	2.12	0.65
1:B:341:GLN:NE2	1:B:349:LEU:O	2.23	0.64
1:C:283:TYR:HB3	1:C:393:LYS:O	1.96	0.64
1:A:50:GLY:HA3	1:A:456:MET:HE1	1.79	0.64
1:B:253:LEU:O	1:B:254:CYS:HB2	1.96	0.64
1:D:365:VAL:HG11	1:D:420[A]:ILE:HD12	1.78	0.64

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:LYS:HA	1:A:315:VAL:O	1.98	0.64
1:A:408:LYS:HD3	4:A:531:MO7:O19	1.98	0.63
1:B:409:TYR:HB3	1:B:413:TYR:HE1	1.63	0.63
1:A:378:SER:HB2	1:A:382:LYS:HE3	1.81	0.63
1:B:368:PHE:CG	1:B:413:TYR:HE2	2.16	0.63
1:A:174:GLU:OE2	1:A:219:GLN:NE2	2.32	0.62
1:A:279:ASP:OD1	1:A:280:PRO:HD2	1.97	0.62
1:D:239:ARG:HA	1:D:243:THR:O	1.99	0.62
1:C:181:THR:HG23	1:C:453:LEU:HB3	1.82	0.62
1:D:279:ASP:OD1	1:D:280:PRO:HD2	1.99	0.62
4:C:531[B]:MO7:MO6	4:C:531[B]:MO7:O21	1.70	0.62
1:C:51:ILE:HB	1:C:126:VAL:HG22	1.83	0.61
1:C:225:LEU:HG	1:C:353:GLN:HE21	1.60	0.61
4:C:531[B]:MO7:O11	4:C:531[B]:MO7:O14	2.17	0.61
4:C:531[B]:MO7:MO7	4:C:531[B]:MO7:O23	1.71	0.61
4:A:531:MO7:MO4	4:A:531:MO7:O14	1.72	0.61
4:B:531[A]:MO7:O23	4:B:531[A]:MO7:MO7	1.71	0.61
1:A:262[B]:TRP:HE3	1:A:295:LEU:HD13	1.65	0.61
1:A:173:GLU:OE1	1:B:233:GLU:HB2	2.00	0.61
4:D:531:MO7:O23	4:D:531:MO7:MO7	1.72	0.61
1:D:408:LYS:NZ	4:D:531:MO7:O23	2.34	0.61
1:B:209:GLY:HA3	1:B:356:PHE:CD2	2.36	0.61
1:B:409:TYR:O	1:B:413:TYR:HD1	1.84	0.60
1:B:184:TYR:CD2	1:B:457:LEU:HD21	2.35	0.60
1:C:188:ARG:HH11	1:C:188:ARG:HG2	1.66	0.60
1:A:284:PRO:HD3	1:A:319:GLY:HA3	1.83	0.60
1:C:57:SER:HA	2:C:503:CL:CL	2.38	0.60
4:B:531[A]:MO7:O22	4:B:531[A]:MO7:MO6	1.72	0.60
1:C:367:ASP:OD2	1:C:371:LYS:HE3	2.00	0.60
1:D:320:ASP:HB3	1:D:323:GLN:NE2	2.17	0.60
4:A:531:MO7:O21	4:A:531:MO7:MO6	1.73	0.60
4:B:531[A]:MO7:O18	4:B:531[A]:MO7:MO6	1.72	0.60
4:C:531[B]:MO7:MO4	4:C:531[B]:MO7:O14	1.73	0.60
4:C:531[B]:MO7:MO2	4:C:531[B]:MO7:O6	1.73	0.60
4:D:531:MO7:O14	4:D:531:MO7:MO4	1.72	0.60
1:A:270:GLN:O	1:A:273:SER:OG	2.12	0.60
1:A:366:MET:HE2	3:A:511:ACY:CH3	2.28	0.59
1:A:230:GLU:O	1:A:232:PRO:HD3	2.01	0.59
4:A:531:MO7:O11	4:A:531:MO7:MO3	1.72	0.59
1:C:239:ARG:NH1	1:C:242:GLY:HA2	2.16	0.59
1:C:239:ARG:HA	1:C:243:THR:O	2.03	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:LEU:HB2	1:D:188:ARG:HG2	1.85	0.59
4:B:531[A]:MO7:MO3	4:B:531[A]:MO7:O11	1.73	0.59
4:B:531[A]:MO7:MO4	4:B:531[A]:MO7:O14	1.72	0.59
1:C:225:LEU:HG	1:C:353:GLN:HE22	1.62	0.59
1:B:409:TYR:O	1:B:413:TYR:CD1	2.56	0.58
1:D:396:GLU:HG2	2:D:508:CL:CL	2.40	0.58
1:A:262[B]:TRP:HE3	1:A:295:LEU:CD1	2.15	0.58
1:B:368:PHE:CD1	1:B:413:TYR:CD2	2.91	0.58
1:B:321:TYR:HB3	1:B:388:LYS:HG3	1.85	0.58
4:D:531:MO7:MO3	4:D:531:MO7:O11	1.73	0.58
1:A:187:GLY:O	1:A:190:LYS:HD2	2.04	0.57
1:C:303:ARG:HD3	1:D:338:PRO:O	2.04	0.57
1:B:407:GLU:OE2	4:C:531[B]:MO7:O21	2.21	0.57
1:D:321:TYR:HB3	1:D:388:LYS:HG2	1.85	0.57
1:A:230:GLU:HB3	1:A:232:PRO:CD	2.34	0.57
1:B:453:LEU:O	1:B:456:MET:HB3	2.05	0.56
1:C:177:TYR:OH	1:C:458:ASN:ND2	2.32	0.56
1:C:381:GLU:O	1:C:385:GLU:HG2	2.07	0.55
1:A:174:GLU:OE2	1:A:219:GLN:CD	2.44	0.55
1:B:341:GLN:HG2	1:B:349:LEU:O	2.06	0.55
1:D:52:VAL:CG2	1:D:456:MET:HE3	2.37	0.55
1:C:253:LEU:O	1:C:254:CYS:HB2	2.08	0.54
1:B:407:GLU:CG	4:C:531[B]:MO7:O21	2.56	0.54
1:A:320:ASP:OD1	1:A:322:GLU:HB2	2.07	0.54
1:B:425:LEU:O	1:B:429:ASN:HA	2.07	0.54
1:C:368:PHE:CE2	1:C:372:MET:CE	2.91	0.54
1:A:326:GLN:OE1	1:A:326:GLN:HA	2.07	0.54
1:D:232:PRO:HD2	2:D:507:CL:CL	2.45	0.54
1:A:263:GLN:OE1	1:A:303:ARG:NH1	2.42	0.53
1:C:395:TRP:CE2	1:C:399:LYS:HE2	2.44	0.53
1:D:228:THR:HB	1:D:351:PRO:HD2	1.91	0.53
1:B:320:ASP:HB3	1:B:323:GLN:NE2	2.24	0.53
1:A:248:TYR:CD1	1:A:248:TYR:C	2.83	0.52
1:C:428:TYR:O	1:C:429:ASN:HB2	2.09	0.52
4:A:531:MO7:O23	4:A:531:MO7:O21	2.27	0.52
1:A:216:SER:HA	1:A:259:GLN:HG2	1.90	0.52
1:D:259:GLN:O	1:D:263:GLN:HG3	2.09	0.52
1:B:368:PHE:CD1	1:B:413:TYR:HD2	2.28	0.52
1:C:320:ASP:HB3	1:C:323:GLN:HE21	1.76	0.51
1:A:230:GLU:HA	1:A:230:GLU:OE1	2.10	0.51
1:B:338:PRO:HG2	1:B:339:TYR:CE2	2.46	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LEU:O	1:A:254:CYS:HB2	2.11	0.51
1:C:458:ASN:HA	1:C:463:ILE:HD11	1.92	0.51
1:A:230:GLU:HB3	1:A:232:PRO:HD3	1.91	0.50
1:C:284:PRO:HD3	1:C:319:GLY:HA3	1.92	0.50
1:A:99:ASP:N	1:A:99:ASP:OD1	2.42	0.50
1:A:83:GLU:HG2	1:A:84:CYS:N	2.27	0.50
1:A:322:GLU:OE1	1:A:322:GLU:HA	2.11	0.49
1:A:177:TYR:CE2	1:A:455:TYR:HD2	2.30	0.49
1:C:332:PHE:CE2	3:C:512:ACY:H3	2.47	0.49
4:D:531:MO7:O6	4:D:531:MO7:O10	2.30	0.49
1:D:370:LYS:HE2	1:D:377:VAL:CB	2.43	0.49
1:C:188:ARG:NH1	1:C:188:ARG:CG	2.65	0.49
1:D:225:LEU:CD1	1:D:353:GLN:HE21	1.93	0.49
1:B:239:ARG:HA	1:B:243:THR:O	2.13	0.49
1:D:240:LEU:O	1:D:241:TYR:HB2	2.13	0.49
1:A:235:SER:O	1:A:236:LEU:HD23	2.12	0.49
1:C:357:GLY:HA2	1:C:439:HIS:O	2.13	0.49
1:D:417:GLY:O	3:D:511:ACY:H3	2.14	0.48
1:A:228:THR:CB	1:B:139:MET:HG2	2.43	0.48
1:C:395:TRP:NE1	1:C:399:LYS:HE2	2.28	0.48
1:B:407:GLU:HG3	4:C:531[B]:MO7:O21	2.14	0.48
1:D:368:PHE:CD2	1:D:413:TYR:CD2	3.02	0.48
1:D:87:LYS:HE3	1:D:87:LYS:HB2	1.65	0.48
1:A:228:THR:CB	1:B:139:MET:CG	2.92	0.47
1:B:460:THR:O	1:B:461:ASN:HB2	2.13	0.47
1:D:157:LYS:HE2	1:D:157:LYS:HB3	1.47	0.47
1:B:284:PRO:HD3	1:B:319:GLY:HA3	1.95	0.47
1:D:178:GLY:O	1:D:182:ILE:HG23	2.14	0.47
1:D:99:ASP:OD1	1:D:99:ASP:N	2.44	0.47
1:A:342:CYS:HB3	1:A:347:VAL:O	2.13	0.47
1:C:240:LEU:HB2	1:C:245:TYR:CE2	2.50	0.47
1:B:353:GLN:O	1:B:353:GLN:HG3	2.15	0.47
1:C:188:ARG:NH1	1:C:188:ARG:HG3	2.29	0.47
4:C:531[B]:MO7:O6	4:C:531[B]:MO7:O16	2.32	0.47
1:A:77:VAL:HA	1:A:184:TYR:OH	2.15	0.47
1:C:287:LYS:HA	1:C:315:VAL:O	2.14	0.47
1:B:221:THR:HA	1:B:248:TYR:O	2.15	0.47
1:B:51:ILE:HB	1:B:126:VAL:HG22	1.96	0.47
1:B:140:GLU:HG3	1:B:299:PRO:HG3	1.96	0.47
1:B:167:LYS:HE2	1:B:455:TYR:OH	2.14	0.47
1:B:434:SER:O	1:B:437:GLN:CG	2.62	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:ALA:HB2	1:B:386:ILE:CD1	2.45	0.46
1:A:230:GLU:HB2	1:A:348:PHE:CZ	2.50	0.46
1:B:65:TYR:CE1	1:B:453:LEU:HD13	2.51	0.46
1:A:167:LYS:NZ	1:B:232:PRO:HB2	2.31	0.46
1:B:110:LYS:HZ2	1:B:114:GLU:HG2	1.81	0.46
1:B:92:SER:OG	2:B:503:CL:CL	2.64	0.46
1:C:214:GLY:HA3	2:C:501:CL:CL	2.53	0.46
1:A:368:PHE:CE2	1:A:413:TYR:HD2	2.34	0.46
1:D:429:ASN:C	1:D:431:THR:H	2.19	0.46
1:D:425:LEU:O	1:D:431:THR:HG23	2.16	0.46
1:A:232:PRO:O	1:A:233:GLU:CB	2.64	0.46
1:A:51:ILE:HB	1:A:126:VAL:HG22	1.98	0.45
1:A:167:LYS:HZ2	1:B:232:PRO:HB2	1.82	0.45
1:B:254:CYS:O	1:B:263:GLN:NE2	2.49	0.45
1:C:240:LEU:HB2	1:C:245:TYR:HE2	1.81	0.45
1:D:341:GLN:HG2	1:D:349:LEU:O	2.15	0.45
1:C:322:GLU:O	1:C:325:HIS:HB3	2.16	0.45
1:B:183:ASN:OD1	1:B:207:THR:HB	2.17	0.45
1:C:99:ASP:N	1:C:99:ASP:OD1	2.44	0.45
1:A:269:ILE:HG23	1:A:269:ILE:O	2.16	0.45
4:A:531:MO7:O12	4:A:531:MO7:O16	2.34	0.45
1:A:443:LYS:HE2	1:A:448:ASN:OD1	2.17	0.44
1:A:231:ALA:CB	1:B:139:MET:SD	3.06	0.44
1:C:320:ASP:HB3	1:C:323:GLN:NE2	2.32	0.44
1:C:455:TYR:CE1	1:C:459:LEU:HD11	2.52	0.44
1:C:188:ARG:HD2	1:C:188:ARG:HA	1.72	0.44
1:A:402:TYR:HA	2:A:505:CL:CL	2.55	0.44
1:D:51:ILE:HB	1:D:126:VAL:HG22	2.00	0.44
1:C:87:LYS:HE3	1:C:87:LYS:HB2	1.74	0.44
1:B:87:LYS:HB2	1:B:87:LYS:HE3	1.70	0.44
1:C:321:TYR:HB2	1:C:388:LYS:HA	2.00	0.44
1:B:269:ILE:HG23	1:B:269:ILE:O	2.17	0.44
1:C:302:LYS:HA	1:C:305:GLU:HG3	1.99	0.44
1:C:460:THR:OG1	1:C:462:MET:HG3	2.18	0.44
1:D:394:PRO:O	1:D:397:GLU:HB3	2.18	0.44
1:A:230:GLU:O	1:A:232:PRO:CD	2.62	0.44
1:B:338:PRO:HG2	1:B:339:TYR:CD2	2.53	0.44
1:B:409:TYR:HB3	1:B:413:TYR:CE1	2.49	0.44
1:C:366:MET:HE2	3:C:511:ACY:H1	1.99	0.44
1:A:240:LEU:HD23	1:A:240:LEU:HA	1.52	0.43
1:B:99:ASP:N	1:B:99:ASP:OD1	2.49	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:TYR:O	1:C:125:PRO:HD2	2.18	0.43
1:A:283:TYR:O	1:A:284:PRO:C	2.56	0.43
1:B:279:ASP:OD1	1:B:280:PRO:HD2	2.18	0.43
1:B:283:TYR:O	1:B:284:PRO:C	2.56	0.43
1:B:396:GLU:HG2	2:B:506:CL:CL	2.55	0.43
1:D:111:MET:O	1:D:115:ARG:HB2	2.19	0.43
1:A:457:LEU:HG	1:A:457:LEU:H	1.68	0.43
1:A:368:PHE:CD2	1:A:413:TYR:CD2	3.07	0.43
1:B:320:ASP:OD1	1:B:322:GLU:HB2	2.18	0.43
1:B:209:GLY:HA3	1:B:356:PHE:CE2	2.54	0.43
4:B:531[A]:MO7:O18	4:B:531[A]:MO7:O20	2.37	0.43
1:C:437:GLN:HB3	1:C:437:GLN:HE21	1.66	0.43
1:C:248:TYR:CD1	1:C:248:TYR:C	2.91	0.42
4:D:531:MO7:O24	4:D:531:MO7:O13	2.36	0.42
1:A:252:PHE:CD2	1:A:344:PHE:CZ	3.07	0.42
1:B:277:LEU:HA	1:B:277:LEU:HD12	1.81	0.42
1:B:323:GLN:HB2	1:B:323:GLN:HE21	1.55	0.42
1:C:241:TYR:CE2	1:C:464:PRO:HD2	2.55	0.42
1:A:368:PHE:CD2	1:A:413:TYR:HD2	2.37	0.42
1:B:179:TRP:HA	1:B:210:ALA:HB2	2.01	0.42
1:C:443:LYS:HE3	1:C:446:ASP:HA	2.02	0.42
1:A:185:LEU:O	1:A:445:LYS:HD2	2.20	0.41
1:A:230:GLU:CA	1:A:232:PRO:HD3	2.43	0.41
1:A:269:ILE:CG2	1:A:269:ILE:O	2.68	0.41
1:C:341:GLN:HG2	1:C:349:LEU:O	2.20	0.41
1:D:213:LEU:HD12	1:D:218:THR:HB	2.02	0.41
1:D:443:LYS:HA	1:D:447:SER:O	2.20	0.41
1:A:188:ARG:NH2	1:A:206:SER:O	2.54	0.41
1:D:225:LEU:HA	1:D:225:LEU:HD12	1.78	0.41
1:D:269:ILE:HA	1:D:269:ILE:HD12	1.91	0.41
1:D:335:SER:HB3	1:D:336:HIS:CD2	2.55	0.41
1:B:320:ASP:HB3	1:B:323:GLN:HE21	1.84	0.41
1:A:177:TYR:CE2	1:A:455:TYR:CD2	3.09	0.41
1:A:87:LYS:HE3	1:A:87:LYS:HB2	1.76	0.41
1:D:57:SER:HA	2:D:503:CL:CL	2.58	0.41
1:A:230:GLU:CA	1:A:230:GLU:OE1	2.69	0.41
1:A:181:THR:HG21	1:A:450:GLY:O	2.21	0.41
1:B:253:LEU:O	1:B:254:CYS:CB	2.66	0.41
1:C:263:GLN:HG2	1:C:300:CYS:O	2.21	0.41
1:C:366:MET:HE1	3:C:511:ACY:H1	2.00	0.41
1:A:440:PHE:CD1	1:A:440:PHE:N	2.88	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:LEU:C	1:A:62:LEU:HD23	2.41	0.40
1:C:430:PHE:CG	1:C:438:ILE:HD11	2.56	0.40
1:B:283:TYR:HB3	1:B:393:LYS:O	2.22	0.40
1:B:83:GLU:HG2	1:B:84:CYS:N	2.37	0.40
1:D:164:GLN:HA	1:D:164:GLN:NE2	2.36	0.40
1:D:221:THR:HA	1:D:248:TYR:O	2.22	0.40
1:A:239:ARG:HA	1:A:243:THR:O	2.21	0.40
1:B:48:LYS:O	1:B:66:LYS:HA	2.21	0.40
1:A:352:LEU:HA	1:A:352:LEU:HD23	1.80	0.40
1:B:332:PHE:CZ	3:B:512:ACY:H3	2.56	0.40
1:C:421:LEU:HD23	1:C:421:LEU:HA	1.91	0.40
1:D:334:ASN:OD1	3:D:512:ACY:O	2.40	0.40
1:D:248:TYR:CE2	1:D:350:PRO:HD3	2.56	0.40
1:D:359:PHE:O	1:D:362:PHE:HB2	2.21	0.40
1:A:231:ALA:HB1	1:B:139:MET:SD	2.62	0.40
1:A:262[B]:TRP:CE3	1:A:295:LEU:CD1	3.01	0.40
1:A:228:THR:CB	1:B:139:MET:HG3	2.51	0.40
1:C:179:TRP:HB2	1:C:221:THR:HG21	2.04	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	377/452 (83%)	348 (92%)	27 (7%)	2 (0%)	32	53
1	B	375/452 (83%)	347 (92%)	26 (7%)	2 (0%)	32	53
1	C	387/452 (86%)	374 (97%)	12 (3%)	1 (0%)	44	66
1	D	394/452 (87%)	370 (94%)	21 (5%)	3 (1%)	22	39
All	All	1533/1808 (85%)	1439 (94%)	86 (6%)	8 (0%)	32	53

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	343	ALA
1	D	226	ASN
1	A	229	LEU
1	D	343	ALA
1	A	227	SER
1	B	188	ARG
1	C	343	ALA
1	D	427	GLY

### 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	318/390 (82%)	291 (92%)	27 (8%)	12	23
1	B	312/390 (80%)	293 (94%)	19 (6%)	22	40
1	C	334/390 (86%)	310 (93%)	24 (7%)	17	31
1	D	330/390 (85%)	311 (94%)	19 (6%)	23	43
All	All	1294/1560 (83%)	1205 (93%)	89 (7%)	18	34

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	SER
1	A	123	GLN
1	A	142	LYS
1	A	154	ARG
1	A	190	LYS
1	A	206	SER
1	A	227	SER
1	A	230	GLU
1	A	235	SER
1	A	237	GLN
1	A	240	LEU
1	A	272	SER
1	A	302	LYS
1	A	303	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	326	GLN
1	A	333	ASN
1	A	340	SER
1	A	353	GLN
1	A	378	SER
1	A	385	GLU
1	A	392	SER
1	A	422	SER
1	A	436	ASP
1	A	437	GLN
1	A	445	LYS
1	A	460	THR
1	A	462	MET
1	B	58	SER
1	B	123	GLN
1	B	142	LYS
1	B	298	THR
1	B	310	PHE
1	B	312	GLN
1	B	322	GLU
1	B	337	CYS
1	B	350	PRO
1	B	353	GLN
1	B	374	ASN
1	B	378	SER
1	B	383	MET
1	B	392	SER
1	B	420	ILE
1	B	422	SER
1	B	436	ASP
1	B	447	SER
1	B	457	LEU
1	C	47	VAL
1	C	58	SER
1	C	59	HIS
1	C	123	GLN
1	C	142	LYS
1	C	154	ARG
1	C	188	ARG
1	C	218	THR
1	C	239	ARG
1	C	244	ASP

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	271	VAL
1	C	272	SER
1	C	290	VAL
1	C	293	SER
1	C	310	PHE
1	C	371	LYS
1	C	381	GLU
1	C	385	GLU
1	C	388	LYS
1	C	392	SER
1	C	437	GLN
1	C	443	LYS
1	C	456	MET
1	C	463	ILE
1	D	58	SER
1	D	99	ASP
1	D	123	GLN
1	D	142	LYS
1	D	225	LEU
1	D	238	PHE
1	D	244	ASP
1	D	272	SER
1	D	298	THR
1	D	310	PHE
1	D	312	GLN
1	D	322	GLU
1	D	333	ASN
1	D	335	SER
1	D	353	GLN
1	D	388	LYS
1	D	392	SER
1	D	433	THR
1	D	462	MET

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

Mol	Chain	Res	Type
1	A	123	GLN
1	A	164	GLN
1	A	172	GLN
1	A	226	ASN
1	A	237	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	250	HIS
1	A	323	GLN
1	A	353	GLN
1	B	85	GLN
1	B	123	GLN
1	B	164	GLN
1	B	250	HIS
1	B	323	GLN
1	B	325	HIS
1	B	374	ASN
1	C	59	HIS
1	C	123	GLN
1	C	164	GLN
1	C	250	HIS
1	C	323	GLN
1	C	353	GLN
1	C	437	GLN
1	C	458	ASN
1	D	61	ASN
1	D	123	GLN
1	D	164	GLN
1	D	250	HIS
1	D	323	GLN
1	D	336	HIS
1	D	353	GLN
1	D	448	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 37 ligands modelled in this entry, 26 are monoatomic - leaving 11 for Mogul analysis.

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
3	ACY	A	511	-	1,3,3	4.21	1 (100%)	0,3,3	0.00	-
4	MO7	A	531	-	24,42,42	4.77	11 (45%)	0,131,131	0.00	-
3	ACY	B	511	-	1,3,3	3.28	1 (100%)	0,3,3	0.00	-
3	ACY	B	512	-	1,3,3	1.83	0	0,3,3	0.00	-
4	MO7	B	531[A]	-	24,42,42	8.39	9 (37%)	0,131,131	0.00	-
3	ACY	C	511	-	1,3,3	3.15	1 (100%)	0,3,3	0.00	-
3	ACY	C	512	-	1,3,3	3.24	1 (100%)	0,3,3	0.00	-
4	MO7	C	531[B]	1	24,42,42	52.02	8 (33%)	0,131,131	0.00	-
3	ACY	D	511	-	1,3,3	0.59	0	0,3,3	0.00	-
3	ACY	D	512	-	1,3,3	1.44	0	0,3,3	0.00	-
4	MO7	D	531	-	24,42,42	7.40	10 (41%)	0,131,131	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
3	ACY	A	511	-	-	0/0/0/0	0/0/0/0
4	MO7	A	531	-	-	0/0/260/260	0/0/12/12
3	ACY	B	511	-	-	0/0/0/0	0/0/0/0
3	ACY	B	512	-	-	0/0/0/0	0/0/0/0
4	MO7	B	531[A]	-	-	0/0/260/260	0/0/12/12
3	ACY	C	511	-	-	0/0/0/0	0/0/0/0
3	ACY	C	512	-	-	0/0/0/0	0/0/0/0
4	MO7	C	531[B]	1	-	0/0/260/260	0/0/12/12
3	ACY	D	511	-	-	0/0/0/0	0/0/0/0
3	ACY	D	512	-	-	0/0/0/0	0/0/0/0
4	MO7	D	531	-	-	0/0/260/260	0/0/12/12

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	531[A]	MO7	O18-MO6	-3.46	1.72	1.93
4	A	531	MO7	O12-MO4	-2.65	1.77	1.93
4	D	531	MO7	O1-MO1	2.04	1.76	1.74
4	A	531	MO7	O1-MO1	2.13	1.76	1.74
4	B	531[A]	MO7	O22-MO6	2.51	1.72	1.68
4	D	531	MO7	O4-MO1	2.61	1.77	1.74
4	D	531	MO7	O23-MO7	2.65	1.72	1.68
4	A	531	MO7	O11-MO3	2.74	1.72	1.68
4	B	531[A]	MO7	O11-MO3	2.92	1.73	1.68
4	D	531	MO7	O11-MO3	3.10	1.73	1.68
3	C	511	ACY	CH3-C	3.15	1.52	1.48
4	C	531[B]	MO7	O15-MO5	3.20	1.74	1.68
4	B	531[A]	MO7	O8-MO2	3.23	1.74	1.68
3	C	512	ACY	CH3-C	3.24	1.52	1.48
4	C	531[B]	MO7	O11-MO3	3.24	1.73	1.68
4	D	531	MO7	O22-MO6	3.25	1.73	1.68
4	A	531	MO7	O23-MO7	3.26	1.73	1.68
3	B	511	ACY	CH3-C	3.28	1.53	1.48
4	A	531	MO7	O8-MO2	3.35	1.74	1.68
4	A	531	MO7	O15-MO5	3.36	1.74	1.68
4	C	531[B]	MO7	O13-MO4	3.37	1.73	1.68
4	C	531[B]	MO7	O1-MO1	3.58	1.78	1.74
4	B	531[A]	MO7	O13-MO4	3.61	1.74	1.68
4	C	531[B]	MO7	O8-MO2	4.02	1.75	1.68
4	A	531	MO7	O4-MO2	4.08	2.40	1.95
3	A	511	ACY	CH3-C	4.21	1.54	1.48
4	C	531[B]	MO7	O4-MO2	4.25	2.42	1.95
4	B	531[A]	MO7	O15-MO5	4.34	1.76	1.68
4	A	531	MO7	O22-MO6	4.36	1.75	1.68
4	A	531	MO7	O1-MO5	4.38	2.43	1.95
4	D	531	MO7	O8-MO2	4.51	1.76	1.68
4	C	531[B]	MO7	O1-MO5	4.53	2.45	1.95
4	D	531	MO7	O15-MO5	4.56	1.76	1.68
4	D	531	MO7	O13-MO4	4.89	1.76	1.68
4	A	531	MO7	O12-MO5	10.28	3.20	1.91
4	B	531[A]	MO7	O18-MO2	17.20	4.07	1.91
4	A	531	MO7	O13-MO4	18.11	1.97	1.68
4	D	531	MO7	O4-MO2	23.59	4.56	1.95
4	B	531[A]	MO7	O4-MO2	24.23	4.63	1.95
4	D	531	MO7	O1-MO5	25.51	4.77	1.95
4	B	531[A]	MO7	O1-MO5	26.92	4.92	1.95
4	C	531[B]	MO7	O22-MO6	254.62	5.85	1.68

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	511	ACY	3	0
4	A	531	MO7	6	0
3	B	512	ACY	1	0
4	B	531[A]	MO7	8	0
3	C	511	ACY	3	0
3	C	512	ACY	1	0
4	C	531[B]	MO7	13	0
3	D	511	ACY	1	0
3	D	512	ACY	1	0
4	D	531	MO7	7	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	385/452 (85%)	0.59	43 (11%) 6 5	41, 79, 132, 158	0
1	B	386/452 (85%)	0.65	49 (12%) 4 3	54, 79, 128, 162	0
1	C	393/452 (86%)	0.24	34 (8%) 11 11	35, 63, 103, 128	0
1	D	397/452 (87%)	0.01	17 (4%) 36 38	32, 58, 92, 114	0
All	All	1561/1808 (86%)	0.37	143 (9%) 10 9	32, 70, 118, 162	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	47	VAL	9.3
1	A	229	LEU	7.4
1	A	122	HIS	7.1
1	B	77	VAL	6.8
1	A	333	ASN	6.7
1	C	68	PRO	6.5
1	C	47	VAL	5.9
1	A	48	LYS	5.7
1	B	117	PRO	5.7
1	B	234	THR	5.5
1	B	49	TYR	5.4
1	B	242	GLY	5.3
1	A	337	CYS	5.3
1	D	69	ALA	5.1
1	B	239	ARG	5.1
1	C	274	GLY	5.1
1	A	246	THR	5.0
1	A	118	ALA	5.0
1	D	336	HIS	5.0
1	C	77	VAL	4.8
1	D	46	ASN	4.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	243	THR	4.7
1	C	119	SER	4.7
1	A	461	ASN	4.7
1	A	242	GLY	4.7
1	A	127	TYR	4.7
1	C	465	ALA	4.7
1	B	244	ASP	4.6
1	C	271	VAL	4.6
1	C	49	TYR	4.5
1	B	240	LEU	4.5
1	B	245	TYR	4.4
1	B	223	VAL	4.2
1	D	335	SER	4.1
1	B	143	GLN	4.1
1	B	122	HIS	4.1
1	C	464	PRO	4.1
1	A	245	TYR	4.0
1	C	205	GLY	4.0
1	C	118	ALA	4.0
1	B	115	ARG	3.9
1	B	241	TYR	3.8
1	B	340	SER	3.8
1	B	243	THR	3.8
1	A	121	GLN	3.7
1	B	121	GLN	3.7
1	B	48	LYS	3.7
1	A	462	MET	3.7
1	A	119	SER	3.7
1	A	241	TYR	3.6
1	A	382	LYS	3.6
1	C	336	HIS	3.6
1	A	79	GLN	3.5
1	A	247	VAL	3.5
1	A	244	ASP	3.4
1	B	157	LYS	3.4
1	B	68	PRO	3.4
1	C	143	GLN	3.4
1	B	118	ALA	3.3
1	D	273	SER	3.3
1	B	248	TYR	3.2
1	B	291	ASN	3.2
1	C	116	ILE	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	237	GLN	3.1
1	D	242	GLY	3.1
1	B	116	ILE	3.1
1	C	307	LYS	3.1
1	B	333	ASN	3.1
1	D	241	TYR	3.1
1	B	119	SER	3.1
1	B	238	PHE	3.0
1	A	346	GLY	3.0
1	C	117	PRO	3.0
1	A	77	VAL	3.0
1	B	246	THR	3.0
1	A	67	TRP	2.9
1	C	273	SER	2.9
1	A	66	LYS	2.9
1	B	189	PHE	2.9
1	C	270	GLN	2.9
1	A	416	SER	2.9
1	B	127	TYR	2.9
1	A	187	GLY	2.8
1	A	102	ALA	2.8
1	D	377	VAL	2.8
1	C	160	PRO	2.8
1	A	385	GLU	2.7
1	C	308	LEU	2.7
1	B	67	TRP	2.7
1	C	96	GLN	2.7
1	B	161	PHE	2.6
1	A	100	GLU	2.6
1	D	272	SER	2.6
1	C	122	HIS	2.6
1	A	338	PRO	2.6
1	D	310	PHE	2.6
1	B	158	SER	2.5
1	D	226	ASN	2.5
1	A	433	THR	2.5
1	A	49	TYR	2.5
1	D	289	VAL	2.5
1	A	340	SER	2.5
1	A	240	LEU	2.5
1	D	311	ASN	2.5
1	A	342	CYS	2.4

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	47	VAL	2.4
1	A	228	THR	2.4
1	C	310	PHE	2.4
1	B	289	VAL	2.4
1	C	157	LYS	2.4
1	B	260	ALA	2.4
1	B	452	THR	2.4
1	B	294	GLU	2.4
1	A	120	LYS	2.4
1	B	120	LYS	2.4
1	C	373	ALA	2.3
1	A	189	PHE	2.3
1	A	339	TYR	2.2
1	D	445	LYS	2.2
1	B	451	TRP	2.2
1	C	407	GLU	2.2
1	A	126	VAL	2.2
1	B	247	VAL	2.2
1	D	243	THR	2.2
1	C	335	SER	2.2
1	A	123	GLN	2.1
1	B	312	GLN	2.1
1	B	385	GLU	2.1
1	C	309	PRO	2.1
1	C	142	LYS	2.1
1	D	271	VAL	2.1
1	B	114	GLU	2.1
1	C	406	LYS	2.1
1	B	435	TRP	2.1
1	B	450	GLY	2.1
1	B	147	GLU	2.1
1	B	79	GLN	2.0
1	C	311	ASN	2.0
1	B	140	GLU	2.0
1	C	462	MET	2.0
1	A	358	ALA	2.0
1	C	463	ILE	2.0
1	C	381	GLU	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 ⓘ

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	ACY	B	512	4/4	0.95	0.64	21.70	61,66,67,67	0
3	ACY	B	511	4/4	0.97	0.29	4.13	45,55,58,59	0
3	ACY	C	512	4/4	0.97	0.22	2.60	33,45,47,49	0
2	CL	B	506	1/1	0.92	0.16	1.56	67,67,67,67	0
2	CL	D	506	1/1	0.97	0.13	0.87	58,58,58,58	0
3	ACY	D	512	4/4	0.98	0.16	0.67	42,42,42,43	0
2	CL	D	501	1/1	0.98	0.18	0.54	41,41,41,41	0
2	CL	D	508	1/1	0.95	0.16	0.50	69,69,69,69	0
2	CL	C	501	1/1	0.98	0.15	-0.39	39,39,39,39	0
3	ACY	C	511	4/4	0.98	0.11	-0.76	29,38,41,45	0
5	NA	B	521	1/1	0.98	0.13	-0.84	56,56,56,56	0
3	ACY	A	511	4/4	0.92	0.14	-0.98	48,54,59,61	0
2	CL	A	501	1/1	0.97	0.13	-1.06	56,56,56,56	0
2	CL	C	503	1/1	0.98	0.08	-1.50	63,63,63,63	0
2	CL	A	505	1/1	0.99	0.11	-1.51	56,56,56,56	0
5	NA	D	521	1/1	0.91	0.07	-1.90	48,48,48,48	0
2	CL	B	505	1/1	0.98	0.04	-1.92	58,58,58,58	0
2	CL	C	505	1/1	0.97	0.06	-2.24	50,50,50,50	0
4	MO7	C	531[B]	31/31	0.98	0.07	-2.34	47,61,73,84	31
2	CL	D	503	1/1	0.98	0.05	-2.42	44,44,44,44	0
3	ACY	D	511	4/4	0.99	0.09	-2.63	45,46,46,52	0
4	MO7	A	531	31/31	0.99	0.06	-2.64	30,43,52,60	31
5	NA	C	522	1/1	0.90	0.05	-2.89	42,42,42,42	0
4	MO7	D	531	31/31	0.99	0.06	-2.90	29,41,54,55	31
2	CL	B	501	1/1	0.97	0.11	-2.91	63,63,63,63	0
4	MO7	B	531[A]	31/31	0.98	0.06	-2.97	43,64,82,94	31
2	CL	A	503	1/1	0.98	0.07	-3.11	60,60,60,60	0
2	CL	B	503	1/1	0.96	0.07	-3.36	65,65,65,65	0
2	CL	B	502	1/1	0.97	0.07	-3.52	60,60,60,60	0
2	CL	D	502	1/1	0.98	0.09	-5.81	52,52,52,52	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CL	D	505	1/1	0.97	0.07	-	58,58,58,58	0
2	CL	A	502	1/1	0.97	0.14	-	60,60,60,60	0
2	CL	C	502	1/1	0.99	0.09	-	54,54,54,54	0
2	CL	D	509	1/1	0.99	0.26	-	42,42,42,42	1
2	CL	C	506	1/1	0.96	0.13	-	43,43,43,43	0
2	CL	D	507	1/1	0.98	0.08	-	52,52,52,52	0
5	NA	C	521	1/1	0.93	0.26	-	58,58,58,58	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.