



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:05 PM GMT

PDB ID : 3SQ8  
Title : Crystal Structure Analysis of the Yeast Tyrosyl-DNA Phosphodiesterase 1  
H432R Mutant (SCAN1 Mutant)  
Authors : Gajewski, S.; White, S.W.  
Deposited on : 2011-07-05  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

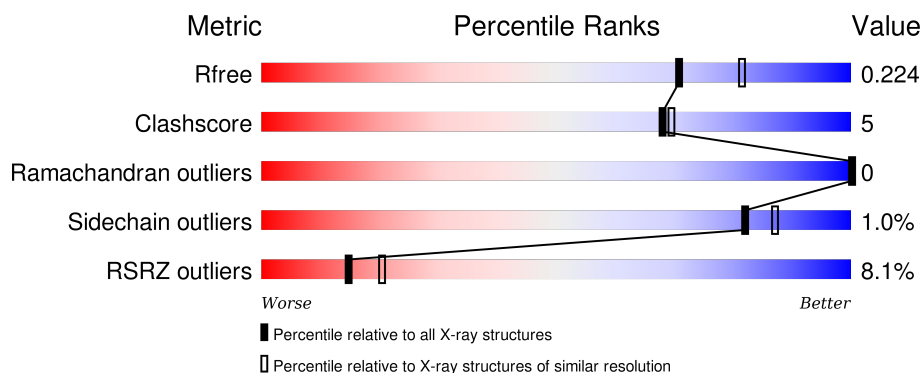
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	470	<div> <div>5%</div> <div>81% 9% 10%</div> </div>
1	B	470	<div> <div>6%</div> <div>80% 10% 10%</div> </div>
1	C	470	<div> <div>9%</div> <div>80% 10% 10%</div> </div>
1	D	470	<div> <div>9%</div> <div>80% 10% 10%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14246 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 Tyrosyl-DNA phosphodiesterase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	P	S	0	0	0
			3430	2223	564	622	1	20			
1	B	423	Total	C	N	O	P	S	0	1	0
			3450	2235	570	624	1	20			
1	C	423	Total	C	N	O	P	S	0	0	0
			3437	2227	565	624	1	20			
1	D	425	Total	C	N	O	P	S	0	1	0
			3457	2241	569	626	1	20			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	MET	-	INITIATING METHIONINE	UNP P38319
A	432	ARG	HIS	ENGINEERED MUTATION	UNP P38319
A	540	LEU	-	EXPRESSION TAG	UNP P38319
A	541	HIS	-	EXPRESSION TAG	UNP P38319
A	542	HIS	-	EXPRESSION TAG	UNP P38319
A	543	HIS	-	EXPRESSION TAG	UNP P38319
A	544	HIS	-	EXPRESSION TAG	UNP P38319
A	545	HIS	-	EXPRESSION TAG	UNP P38319
A	546	HIS	-	EXPRESSION TAG	UNP P38319
A	547	HIS	-	EXPRESSION TAG	UNP P38319
B	78	MET	-	INITIATING METHIONINE	UNP P38319
B	432	ARG	HIS	ENGINEERED MUTATION	UNP P38319
B	540	LEU	-	EXPRESSION TAG	UNP P38319
B	541	HIS	-	EXPRESSION TAG	UNP P38319
B	542	HIS	-	EXPRESSION TAG	UNP P38319
B	543	HIS	-	EXPRESSION TAG	UNP P38319
B	544	HIS	-	EXPRESSION TAG	UNP P38319
B	545	HIS	-	EXPRESSION TAG	UNP P38319
B	546	HIS	-	EXPRESSION TAG	UNP P38319
B	547	HIS	-	EXPRESSION TAG	UNP P38319
C	78	MET	-	INITIATING METHIONINE	UNP P38319

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Chain	Residue	Modelled	Actual	Comment	Reference
C	432	ARG	HIS	ENGINEERED MUTATION	UNP P38319
C	540	LEU	-	EXPRESSION TAG	UNP P38319
C	541	HIS	-	EXPRESSION TAG	UNP P38319
C	542	HIS	-	EXPRESSION TAG	UNP P38319
C	543	HIS	-	EXPRESSION TAG	UNP P38319
C	544	HIS	-	EXPRESSION TAG	UNP P38319
C	545	HIS	-	EXPRESSION TAG	UNP P38319
C	546	HIS	-	EXPRESSION TAG	UNP P38319
C	547	HIS	-	EXPRESSION TAG	UNP P38319
D	78	MET	-	INITIATING METHIONINE	UNP P38319
D	432	ARG	HIS	ENGINEERED MUTATION	UNP P38319
D	540	LEU	-	EXPRESSION TAG	UNP P38319
D	541	HIS	-	EXPRESSION TAG	UNP P38319
D	542	HIS	-	EXPRESSION TAG	UNP P38319
D	543	HIS	-	EXPRESSION TAG	UNP P38319
D	544	HIS	-	EXPRESSION TAG	UNP P38319
D	545	HIS	-	EXPRESSION TAG	UNP P38319
D	546	HIS	-	EXPRESSION TAG	UNP P38319
D	547	HIS	-	EXPRESSION TAG	UNP P38319

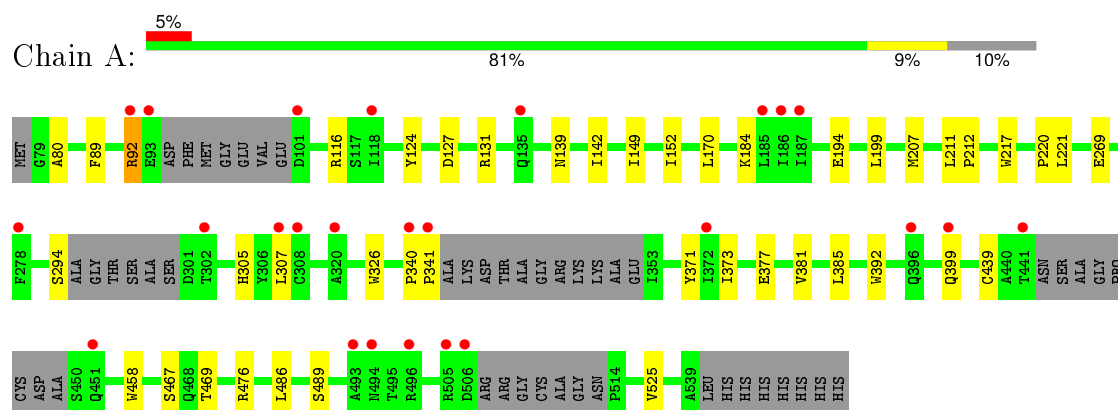
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	168	Total O 168 168	0	0
2	B	146	Total O 146 146	0	0
2	C	95	Total O 95 95	0	0
2	D	63	Total O 63 63	0	0

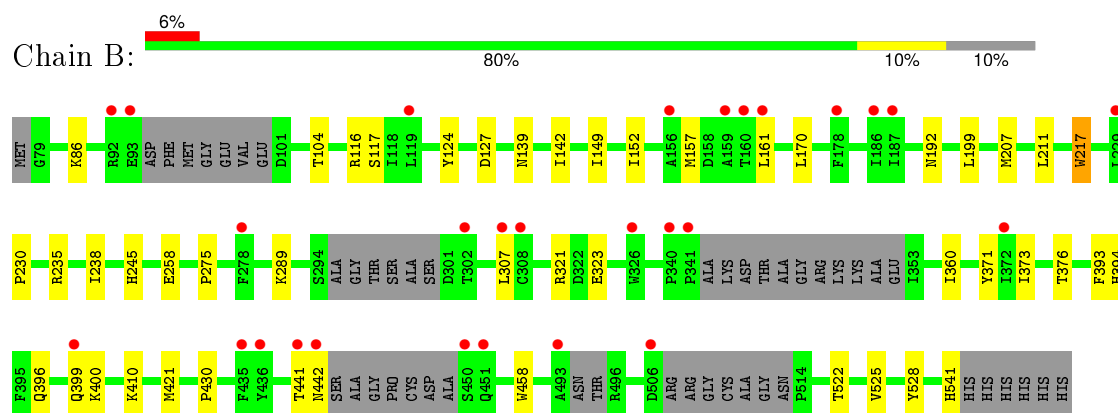
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

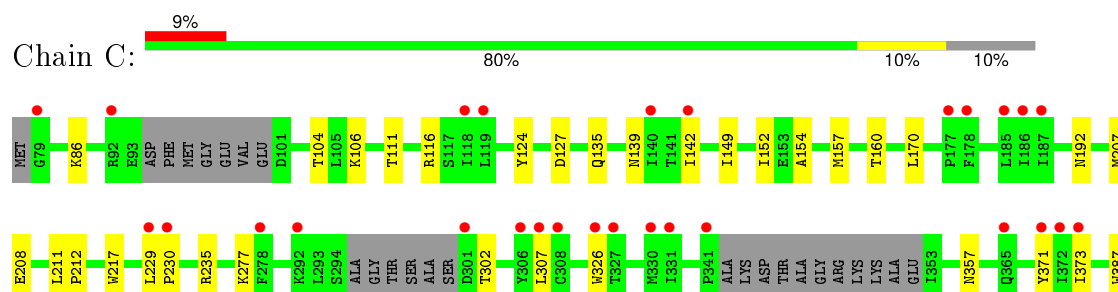
#### • Molecule 1: Tyrosyl-DNA phosphodiesterase 1

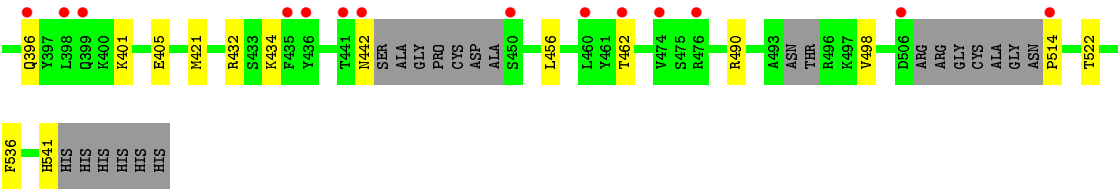


#### • Molecule 1: Tyrosyl-DNA phosphodiesterase 1

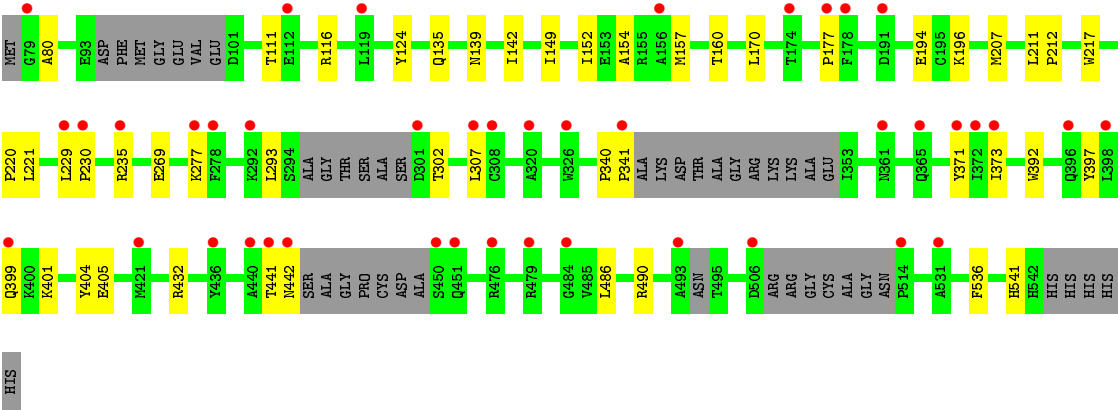
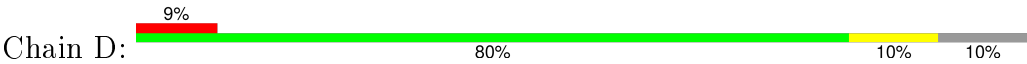


#### • Molecule 1: Tyrosyl-DNA phosphodiesterase 1





● Molecule 1: Tyrosyl-DNA phosphodiesterase 1



HIS

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.87Å 81.49Å 96.79Å 89.52° 84.90° 67.82°	Depositor
Resolution (Å)	24.79 – 2.10 24.79 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.4 (24.79-2.10) 93.0 (24.79-2.10)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.38 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.187 , 0.226 0.183 , 0.224	Depositor DCC
$R_{free}$ test set	4912 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.7	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 42.8	EDS
Estimated twinning fraction	0.003 for -h,-h+k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 98039 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14246	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NEP

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	0.64	4/3501 (0.1%)	0.69	0/4734
1	B	0.65	2/3525 (0.1%)	0.68	0/4765
1	C	0.58	3/3508 (0.1%)	0.63	1/4743 (0.0%)
1	D	0.55	1/3532 (0.0%)	0.61	0/4776
All	All	0.60	10/14066 (0.1%)	0.66	1/19018 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	326	TRP	CD2-CE2	5.68	1.48	1.41
1	A	458	TRP	CD2-CE2	5.60	1.48	1.41
1	B	458	TRP	CD2-CE2	5.43	1.47	1.41
1	A	217	TRP	CD2-CE2	5.38	1.47	1.41
1	A	392	TRP	CD2-CE2	5.36	1.47	1.41
1	C	217	TRP	CD2-CE2	5.35	1.47	1.41
1	C	387	TRP	CD2-CE2	5.34	1.47	1.41
1	B	217	TRP	CD2-CE2	5.32	1.47	1.41
1	C	326	TRP	CD2-CE2	5.28	1.47	1.41
1	D	217	TRP	CD2-CE2	5.13	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	432	ARG	NE-CZ-NH2	-5.51	117.54	120.30

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	3430	0	3419	28	0
1	B	3450	0	3436	46	0
1	C	3437	0	3418	29	0
1	D	3457	0	3438	41	0
2	A	168	0	0	2	0
2	B	146	0	0	2	0
2	C	95	0	0	3	0
2	D	63	0	0	1	0
All	All	14246	0	13711	128	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 5.

All (128) 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:B:207:MET:HE2	1:D:541:HIS:HE1	1.26	0.99
1:B:149:ILE:HD13	1:B:170:LEU:HD11	1.44	0.96
1:D:149:ILE:HD13	1:D:170:LEU:HD11	1.48	0.96
1:C:149:ILE:HD13	1:C:170:LEU:HD11	1.52	0.89
1:C:514:PRO:HD3	1:D:177:PRO:HG3	1.57	0.85
1:A:149:ILE:HD13	1:A:170:LEU:HD11	1.61	0.82
1:B:541:HIS:HE1	1:D:207:MET:HE2	1.45	0.80
1:B:207:MET:CE	1:D:541:HIS:HE1	1.96	0.78
1:B:149:ILE:CD1	1:B:170:LEU:HD11	2.15	0.76
1:B:207:MET:HE2	1:D:541:HIS:CE1	2.18	0.75
1:B:207:MET:HE1	1:B:211:LEU:HD11	1.72	0.72
1:B:207:MET:CE	1:B:211:LEU:HD11	2.22	0.69
1:C:302:THR:HG22	1:C:442:ASN:HB2	1.74	0.69
1:A:149:ILE:CD1	1:A:170:LEU:HD11	2.25	0.67
1:B:541:HIS:HE1	1:D:207:MET:CE	2.08	0.66
1:B:207:MET:CE	1:D:541:HIS:CE1	2.76	0.66
1:D:441:THR:O	1:D:442:ASN:HB2	1.96	0.65
1:C:149:ILE:CD1	1:C:170:LEU:HD11	2.27	0.63
1:B:149:ILE:HD13	1:B:170:LEU:CD1	2.23	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:MET:HE1	1:A:211:LEU:HD11	1.81	0.62
1:C:135:GLN:NE2	1:C:160:THR:HG23	2.13	0.62
1:B:275:PRO:HG2	1:C:229:LEU:HD11	1.80	0.62
1:B:400:LYS:HG2	2:B:615:HOH:O	2.00	0.62
1:D:149:ILE:CD1	1:D:170:LEU:HD11	2.25	0.61
1:B:321:ARG:NH1	1:B:323:GLU:OE2	2.34	0.60
1:C:357:ASN:HB2	2:C:617:HOH:O	2.01	0.60
1:B:116:ARG:HE	1:B:139:ASN:ND2	1.99	0.59
1:D:230:PRO:HA	2:D:560:HOH:O	2.01	0.58
1:B:394[B]:HIS:CE1	1:B:396:GLN:HG2	2.38	0.58
1:D:207:MET:HE1	1:D:211:LEU:HD11	1.87	0.57
1:D:207:MET:CE	1:D:211:LEU:HD11	2.35	0.57
1:C:116:ARG:HE	1:C:139:ASN:ND2	2.02	0.57
1:B:124:TYR:CZ	1:B:142:ILE:HG23	2.40	0.57
1:D:116:ARG:HE	1:D:139:ASN:ND2	2.03	0.57
1:A:207:MET:CE	1:A:211:LEU:HD11	2.36	0.56
1:A:116:ARG:HE	1:A:139:ASN:ND2	2.03	0.56
1:C:127:ASP:HB3	1:C:152:ILE:HG12	1.89	0.55
1:D:269:GLU:HB2	1:D:486:LEU:HB3	1.89	0.55
1:B:541:HIS:CE1	1:D:207:MET:CE	2.88	0.54
1:B:245:HIS:HD2	1:C:229:LEU:CD2	2.20	0.54
1:C:307:LEU:HD11	1:C:373:ILE:HD11	1.90	0.54
1:C:192:ASN:N	1:C:192:ASN:OD1	2.41	0.53
1:C:490:ARG:HB3	2:C:615:HOH:O	2.09	0.53
1:A:127:ASP:HB3	1:A:152:ILE:HG12	1.90	0.53
1:D:149:ILE:HD13	1:D:170:LEU:CD1	2.32	0.53
1:A:467:SER:OG	1:A:469:THR:HG22	2.08	0.53
1:B:360:ILE:HD11	1:B:410:LYS:HB3	1.91	0.52
1:C:401:LYS:O	1:C:405:GLU:HG2	2.09	0.52
1:B:86:LYS:HB3	1:B:104:THR:HG22	1.92	0.52
1:C:207:MET:CE	1:C:211:LEU:HD11	2.40	0.51
1:B:116:ARG:HG3	1:B:139:ASN:HD22	1.76	0.51
1:A:89:PHE:O	1:A:92:ARG:NH1	2.44	0.50
1:D:124:TYR:CZ	1:D:142:ILE:HG23	2.46	0.50
1:B:307:LEU:HD11	1:B:373:ILE:HD11	1.93	0.50
1:C:124:TYR:CZ	1:C:142:ILE:HG23	2.46	0.50
1:C:456:LEU:HB2	1:C:498:VAL:HB	1.92	0.50
1:C:207:MET:HE1	1:C:211:LEU:HD11	1.94	0.49
1:B:289:LYS:HE3	2:B:655:HOH:O	2.12	0.49
1:D:302:THR:HB	1:D:441:THR:O	2.12	0.49
1:B:376:THR:HG22	1:B:528:TYR:CZ	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:THR:O	1:B:442:ASN:HB2	2.13	0.49
1:C:490:ARG:CB	2:C:615:HOH:O	2.61	0.48
1:A:149:ILE:HD13	1:A:170:LEU:CD1	2.39	0.48
1:D:392:TRP:HB3	1:D:432:ARG:HD3	1.94	0.48
1:D:293:LEU:O	1:D:490:ARG:HD3	2.13	0.48
1:D:397:TYR:HB2	1:D:404:TYR:HB2	1.95	0.47
1:D:230:PRO:HB3	1:D:235:ARG:HH21	1.80	0.47
1:A:373:ILE:CD1	1:A:525:VAL:HG11	2.45	0.47
1:D:536:PHE:CE1	1:D:541:HIS:CD2	3.02	0.47
1:B:541:HIS:NE2	1:D:207:MET:HG3	2.30	0.47
1:C:434:LYS:HB2	1:C:462:THR:O	2.14	0.47
1:B:192:ASN:OD1	1:B:192:ASN:N	2.47	0.47
1:B:199:LEU:HD12	1:B:217:TRP:CE3	2.50	0.46
1:B:127:ASP:HB3	1:B:152:ILE:HG12	1.97	0.46
1:D:441:THR:O	1:D:442:ASN:CB	2.62	0.46
1:B:421:MET:CE	1:B:522:THR:HB	2.46	0.45
1:D:135:GLN:NE2	1:D:160:THR:HG23	2.32	0.45
1:A:381:VAL:CG1	1:B:230:PRO:HD3	2.47	0.45
1:A:211:LEU:CD2	1:A:385:LEU:CD1	2.94	0.45
1:D:194:GLU:HB3	1:D:221:LEU:HD11	1.98	0.45
1:B:394[B]:HIS:CE1	1:B:396:GLN:CG	3.00	0.45
1:D:401:LYS:O	1:D:405:GLU:HG2	2.16	0.45
1:D:229:LEU:HA	1:D:230:PRO:HD2	1.79	0.44
1:D:307:LEU:HD11	1:D:373:ILE:HD11	1.99	0.44
1:C:536:PHE:HE1	1:C:541:HIS:CE1	2.36	0.44
1:A:307:LEU:HD11	1:A:373:ILE:HD11	1.98	0.44
1:B:230:PRO:HB3	1:B:235:ARG:HH21	1.83	0.43
1:B:207:MET:HG3	1:D:541:HIS:CE1	2.54	0.43
1:A:381:VAL:HG12	1:B:230:PRO:HD3	1.99	0.43
1:A:124:TYR:CZ	1:A:142:ILE:HG23	2.53	0.43
1:B:393:PHE:CZ	1:B:430:PRO:HB2	2.54	0.43
1:A:194:GLU:CD	1:A:221:LEU:HD21	2.38	0.43
1:A:194:GLU:OE2	1:A:221:LEU:HD21	2.18	0.43
1:D:80:ALA:HB2	1:D:220:PRO:HD3	2.00	0.43
1:C:396:GLN:OE1	1:C:396:GLN:HA	2.19	0.43
1:A:80:ALA:HB2	1:A:220:PRO:HD3	2.00	0.43
1:C:277:LYS:HB2	1:C:277:LYS:HE3	1.65	0.43
1:B:207:MET:HE3	1:B:211:LEU:HD11	2.00	0.43
1:A:127:ASP:O	1:A:131:ARG:HG3	2.19	0.43
1:D:340:PRO:HA	1:D:341:PRO:HD2	1.84	0.43
1:D:211:LEU:HB2	1:D:212:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:MET:HE3	1:B:211:LEU:CD1	2.49	0.42
1:B:541:HIS:HA	1:D:392:TRP:CZ2	2.54	0.42
1:A:116:ARG:HE	1:A:139:ASN:HD22	1.67	0.42
1:A:377:GLU:HG2	2:A:596:HOH:O	2.18	0.42
1:D:277:LYS:HE3	1:D:277:LYS:HB2	1.73	0.42
1:A:184:LYS:O	1:A:199:LEU:HD23	2.19	0.42
1:A:211:LEU:HB2	1:A:212:PRO:HD3	2.02	0.42
1:D:154:ALA:O	1:D:157:MET:HB2	2.20	0.41
1:A:211:LEU:CD2	1:A:385:LEU:HD12	2.50	0.41
1:C:154:ALA:O	1:C:157:MET:HB2	2.20	0.41
1:C:149:ILE:HD13	1:C:170:LEU:CD1	2.37	0.41
1:D:230:PRO:HB3	1:D:235:ARG:NH2	2.35	0.41
1:A:305:HIS:HB2	1:A:439:CYS:HB3	2.03	0.41
1:C:230:PRO:HB3	1:C:235:ARG:HH21	1.86	0.41
1:A:294:SER:HA	2:A:656:HOH:O	2.20	0.41
1:B:541:HIS:CE1	1:D:207:MET:HE2	2.36	0.41
1:B:207:MET:CE	1:B:211:LEU:CD1	2.97	0.40
1:B:207:MET:HB3	1:B:207:MET:HE3	1.95	0.40
1:B:373:ILE:HD13	1:B:525:VAL:HG11	2.02	0.40
1:C:421:MET:SD	1:C:522:THR:HB	2.62	0.40
1:A:269:GLU:HB2	1:A:486:LEU:HB3	2.03	0.40
1:D:152:ILE:HB	1:D:157:MET:HE3	2.03	0.40
1:C:211:LEU:HB2	1:C:212:PRO:CD	2.51	0.40
1:A:340:PRO:HA	1:A:341:PRO:HD2	1.78	0.40
1:C:86:LYS:HB3	1:C:104:THR:HG22	2.04	0.40
1:B:238:ILE:HD13	1:B:258:GLU:OE2	2.21	0.40
1:B:157:MET:CE	1:B:161:LEU:HB3	2.52	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	409/470 (87%)	398 (97%)	11 (3%)	0	100	100
1	B	409/470 (87%)	401 (98%)	8 (2%)	0	100	100
1	C	408/470 (87%)	398 (98%)	10 (2%)	0	100	100
1	D	411/470 (87%)	403 (98%)	8 (2%)	0	100	100
All	All	1637/1880 (87%)	1600 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	383/422 (91%)	378 (99%)	5 (1%)	76	82
1	B	386/422 (92%)	383 (99%)	3 (1%)	86	91
1	C	384/422 (91%)	380 (99%)	4 (1%)	82	87
1	D	386/422 (92%)	382 (99%)	4 (1%)	82	87
All	All	1539/1688 (91%)	1523 (99%)	16 (1%)	82	87

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	ARG
1	A	371	TYR
1	A	399	GLN
1	A	476	ARG
1	A	489	SER
1	B	117	SER
1	B	371	TYR
1	B	399	GLN
1	C	106	LYS
1	C	111	THR
1	C	208	GLU
1	C	371	TYR
1	D	111	THR

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Mol	Chain	Res	Type
1	D	196	LYS
1	D	371	TYR
1	D	399	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
1	A	139	ASN
1	A	242	ASN
1	A	288	ASN
1	B	139	ASN
1	B	242	ASN
1	B	288	ASN
1	B	541	HIS
1	C	135	GLN
1	C	139	ASN
1	C	242	ASN
1	C	288	ASN
1	C	309	GLN
1	D	135	GLN
1	D	139	ASN
1	D	242	ASN
1	D	288	ASN
1	D	541	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	NEP	A	182	1	10,14,15	2.12	5 (50%)	4,20,22	2.65	1 (25%)
1	NEP	B	182	1	10,14,15	2.35	4 (40%)	4,20,22	2.85	2 (50%)
1	NEP	C	182	1	10,14,15	2.34	5 (50%)	4,20,22	2.49	1 (25%)
1	NEP	D	182	1	10,14,15	2.15	4 (40%)	4,20,22	2.78	1 (25%)

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	NEP	A	182	1	-	0/4/12/14	0/1/1/1
1	NEP	B	182	1	-	0/4/12/14	0/1/1/1
1	NEP	C	182	1	-	0/4/12/14	0/1/1/1
1	NEP	D	182	1	-	0/4/12/14	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	182	NEP	CD2-NE2	-4.03	1.32	1.39
1	D	182	NEP	CD2-NE2	-3.61	1.32	1.39
1	C	182	NEP	CD2-NE2	-2.99	1.33	1.39
1	A	182	NEP	CD2-NE2	-2.79	1.34	1.39
1	A	182	NEP	CD2-CG	2.64	1.40	1.36
1	A	182	NEP	P-O2P	2.78	1.60	1.54
1	B	182	NEP	P-O2P	2.81	1.60	1.54
1	D	182	NEP	P-O1P	2.85	1.61	1.54
1	C	182	NEP	P-O2P	2.95	1.61	1.54
1	A	182	NEP	P-O1P	3.08	1.61	1.54
1	D	182	NEP	P-O3P	3.16	1.50	1.47
1	C	182	NEP	CD2-CG	3.17	1.41	1.36
1	D	182	NEP	P-O2P	3.17	1.61	1.54
1	C	182	NEP	P-O3P	3.42	1.50	1.47
1	B	182	NEP	P-O3P	3.43	1.50	1.47
1	A	182	NEP	P-O3P	3.45	1.50	1.47
1	C	182	NEP	P-O1P	3.64	1.62	1.54
1	B	182	NEP	CD2-CG	3.82	1.41	1.36

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	D	182	NEP	CG-CD2-NE2	-5.09	102.15	108.96
1	B	182	NEP	CG-CD2-NE2	-4.61	102.80	108.96
1	A	182	NEP	CG-CD2-NE2	-4.57	102.85	108.96
1	C	182	NEP	CG-CD2-NE2	-4.23	103.30	108.96
1	B	182	NEP	O1P-P-O3P	-2.13	105.60	112.25

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](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	421/470 (89%)	0.08	25 (5%) 26 34	25, 39, 68, 104	0
1	B	422/470 (89%)	0.18	28 (6%) 22 29	25, 40, 72, 103	0
1	C	422/470 (89%)	0.46	42 (9%) 9 13	32, 51, 81, 132	0
1	D	424/470 (90%)	0.50	42 (9%) 9 13	33, 54, 89, 142	0
All	All	1689/1880 (89%)	0.31	137 (8%) 15 20	25, 46, 80, 142	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	341	PRO	10.9
1	D	341	PRO	10.9
1	D	442	ASN	9.6
1	D	178	PHE	7.5
1	C	442	ASN	6.5
1	D	441	THR	6.2
1	A	341	PRO	6.1
1	C	178	PHE	6.0
1	B	442	ASN	5.7
1	B	341	PRO	5.6
1	D	278	PHE	5.5
1	A	340	PRO	5.3
1	D	506	ASP	5.2
1	D	450	SER	5.0
1	C	326	TRP	4.9
1	C	441	THR	4.8
1	D	177	PRO	4.4
1	A	494	ASN	4.3
1	D	277	LYS	4.3
1	C	331	ILE	4.3
1	C	372	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	230	PRO	4.2
1	C	307	LEU	4.1
1	D	320	ALA	3.8
1	D	308	CYS	3.8
1	D	307	LEU	3.7
1	B	278	PHE	3.7
1	C	506	ASP	3.7
1	D	396	GLN	3.7
1	B	93	GLU	3.7
1	C	308	CYS	3.5
1	B	92	ARG	3.4
1	C	399	GLN	3.4
1	D	373	ILE	3.3
1	D	326	TRP	3.3
1	A	493	ALA	3.3
1	B	372	ILE	3.3
1	C	278	PHE	3.3
1	C	373	ILE	3.3
1	A	278	PHE	3.2
1	C	177	PRO	3.2
1	A	441	THR	3.2
1	D	398	LEU	3.2
1	B	156	ALA	3.1
1	C	436	TYR	3.1
1	B	161	LEU	3.1
1	C	119	LEU	3.1
1	B	159	ALA	3.1
1	B	340	PRO	3.1
1	C	229	LEU	3.0
1	B	186	ILE	3.0
1	A	451	GLN	3.0
1	B	308	CYS	3.0
1	A	187	ILE	3.0
1	C	292	LYS	3.0
1	A	320	ALA	2.9
1	B	178	PHE	2.9
1	A	496	ARG	2.9
1	B	307	LEU	2.9
1	A	93	GLU	2.9
1	D	399	GLN	2.9
1	D	440	ALA	2.8
1	C	118	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	396	GLN	2.8
1	D	292	LYS	2.8
1	B	441	THR	2.8
1	D	371	TYR	2.8
1	D	436	TYR	2.8
1	B	326	TRP	2.8
1	C	142	ILE	2.8
1	D	119	LEU	2.8
1	D	531	ALA	2.7
1	C	92	ARG	2.7
1	C	398	LEU	2.7
1	A	506	ASP	2.7
1	C	514	PRO	2.6
1	A	186	ILE	2.6
1	A	92	ARG	2.6
1	C	306	TYR	2.6
1	C	140	ILE	2.6
1	C	330	MET	2.6
1	B	506	ASP	2.6
1	D	79	GLY	2.5
1	A	399	GLN	2.5
1	B	229	LEU	2.5
1	B	187	ILE	2.5
1	B	436	TYR	2.5
1	D	301	ASP	2.5
1	A	308	CYS	2.5
1	D	372	ILE	2.5
1	C	327	THR	2.5
1	B	451	GLN	2.5
1	A	185	LEU	2.5
1	D	230	PRO	2.5
1	B	302	THR	2.5
1	C	396	GLN	2.5
1	D	361	ASN	2.4
1	A	505	ARG	2.4
1	C	476	ARG	2.4
1	D	514	PRO	2.4
1	C	450	SER	2.4
1	D	484	GLY	2.4
1	C	371	TYR	2.4
1	C	365	GLN	2.4
1	A	302	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	372	ILE	2.4
1	D	235	ARG	2.4
1	D	421	MET	2.4
1	A	118	ILE	2.3
1	C	187	ILE	2.3
1	B	450	SER	2.3
1	D	191	ASP	2.3
1	C	186	ILE	2.3
1	C	185	LEU	2.3
1	D	229	LEU	2.3
1	B	160	THR	2.3
1	C	460	LEU	2.3
1	C	301	ASP	2.2
1	B	119	LEU	2.2
1	D	451	GLN	2.2
1	D	476	ARG	2.2
1	B	493	ALA	2.2
1	C	435	PHE	2.2
1	D	493	ALA	2.1
1	D	174	THR	2.1
1	B	435	PHE	2.1
1	C	474	VAL	2.1
1	A	101	ASP	2.1
1	A	307	LEU	2.1
1	A	135	GLN	2.1
1	B	399	GLN	2.1
1	C	79	GLY	2.1
1	D	365	GLN	2.1
1	C	462	THR	2.1
1	D	156	ALA	2.1
1	D	479	ARG	2.1
1	D	112	GLU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	NEP	A	182	14/15	0.97	0.10	-	27,31,32,39	4
1	NEP	D	182	14/15	0.96	0.08	-	38,40,41,47	4
1	NEP	B	182	14/15	0.96	0.09	-	27,29,31,37	4
1	NEP	C	182	14/15	0.96	0.09	-	34,35,37,42	4

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.