



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 03:51 am GMT

PDB ID : 1W0C  
Title : INHIBITION OF LEISHMANIA MAJOR PTERIDINE REDUCTASE (PTR1) BY 2,4,6-TRIAMINOQUINAZOLINE; STRUCTURE OF THE NADP TERNARY COMPLEX.  
Authors : Mcluskey, K.; Gibellini, F.; Carvalho, P.; Avery, M.; Hunter, W.  
Deposited on : 2004-06-02  
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
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)	:	recalc28949

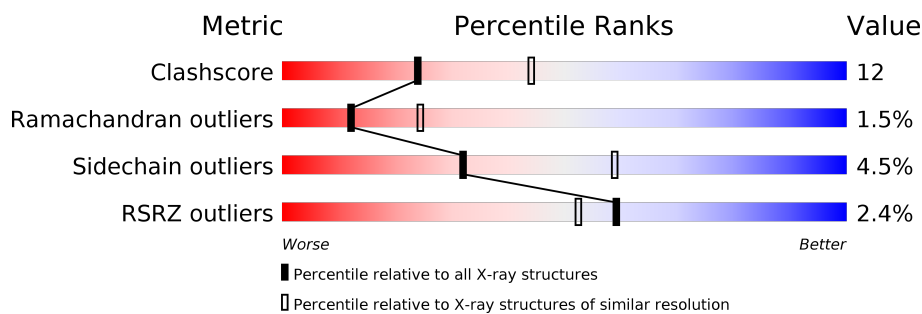
# 1 Overall quality at a glance

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))
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (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	307	<div> <div>69%</div> <div>19%</div> <div>10%</div> </div>
1	B	307	<div> <div>68%</div> <div>18%</div> <div>11%</div> </div>
1	C	307	<div> <div>70%</div> <div>15%</div> <div>14%</div> </div>
1	D	307	<div> <div>66%</div> <div>16%</div> <div>17%</div> </div>
1	E	307	<div> <div>2%</div> <div>65%</div> <div>19%</div> <div>13%</div> </div>
1	F	307	<div> <div>65%</div> <div>20%</div> <div>12%</div> </div>
1	G	307	<div> <div>6%</div> <div>59%</div> <div>23%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
1	H	307	<div><div></div><div>4%</div><div>62%</div><div>21%</div><div>•</div><div>15%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17458 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.

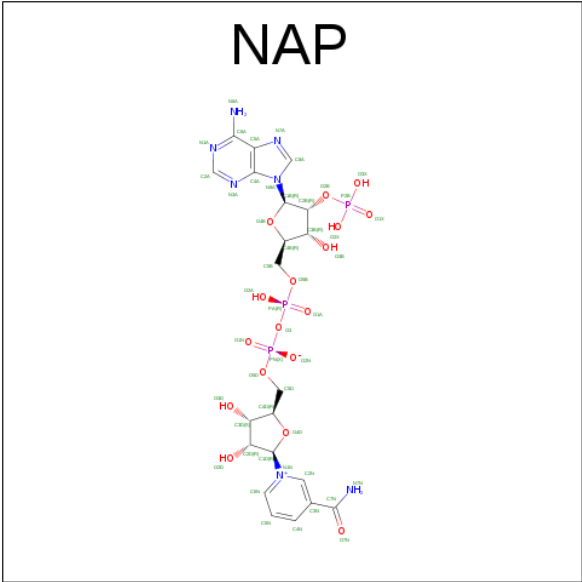
- Molecule 1 is a protein called PTERIDINE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	3	0	0
			2041	1282	361	387	11			
1	B	274	Total	C	N	O	S	3	0	0
			2031	1276	361	383	11			
1	C	264	Total	C	N	O	S	22	0	0
			1954	1227	351	366	10			
1	D	256	Total	C	N	O	S	10	0	0
			1906	1201	342	353	10			
1	E	267	Total	C	N	O	S	0	0	0
			1992	1254	355	372	11			
1	F	270	Total	C	N	O	S	3	0	0
			2013	1265	358	379	11			
1	G	263	Total	C	N	O	S	22	0	0
			1962	1233	350	368	11			
1	H	260	Total	C	N	O	S	10	0	0
			1941	1225	347	359	10			

There are 8 discrepancies between the modelled and reference sequences:

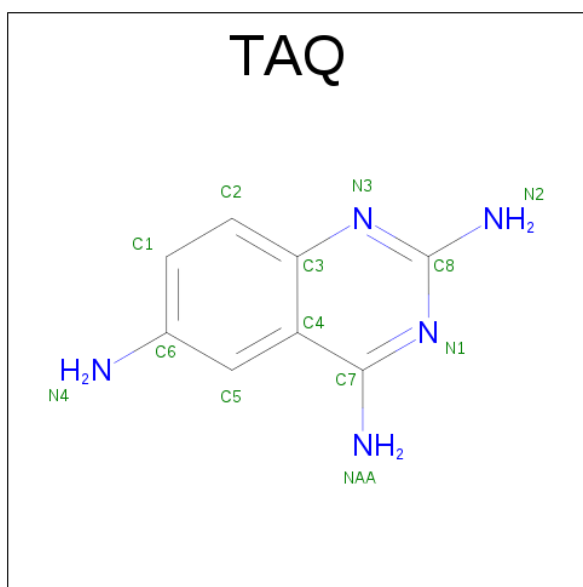
Chain	Residue	Modelled	Actual	Comment	Reference
A	162	VAL	PHE	CONFLICT	UNP Q01782
B	162	VAL	PHE	CONFLICT	UNP Q01782
C	162	VAL	PHE	CONFLICT	UNP Q01782
D	162	VAL	PHE	CONFLICT	UNP Q01782
E	162	VAL	PHE	CONFLICT	UNP Q01782
F	162	VAL	PHE	CONFLICT	UNP Q01782
G	162	VAL	PHE	CONFLICT	UNP Q01782
H	162	VAL	PHE	CONFLICT	UNP Q01782

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 2,4,6-TRIAMINOQUINAZOLINE (three-letter code: TAQ) (formula: C<sub>8</sub>H<sub>9</sub>N<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			13	8	5		
3	A	1	Total	C	N	0	0
			13	8	5		
3	B	1	Total	C	N	0	0
			13	8	5		
3	C	1	Total	C	N	0	0
			13	8	5		
3	D	1	Total	C	N	0	0
			13	8	5		
3	E	1	Total	C	N	0	0
			13	8	5		
3	F	1	Total	C	N	0	0
			13	8	5		
3	G	1	Total	C	N	0	0
			13	8	5		
3	H	1	Total	C	N	0	0
			13	8	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	214	Total	O	0	0
			214	214		
4	B	216	Total	O	0	0
			216	216		
4	C	117	Total	O	0	0
			117	117		

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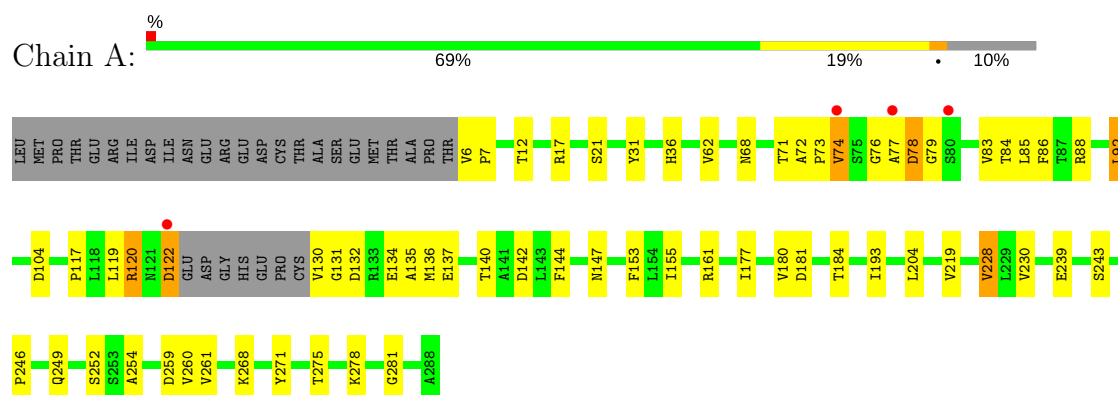
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	97	Total 97	O 97	0	0
4	E	127	Total 127	O 127	0	0
4	F	104	Total 104	O 104	0	0
4	G	143	Total 143	O 143	0	0
4	H	99	Total 99	O 99	0	0

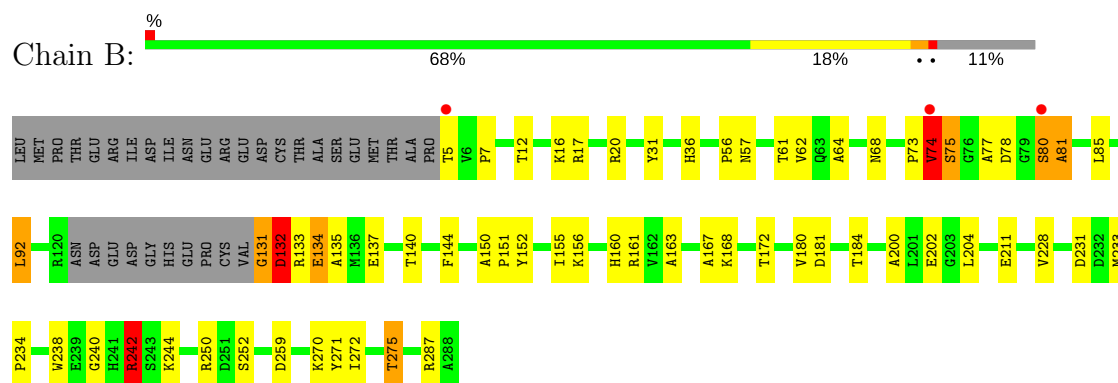
### 3 Residue-property plots [i](#)

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

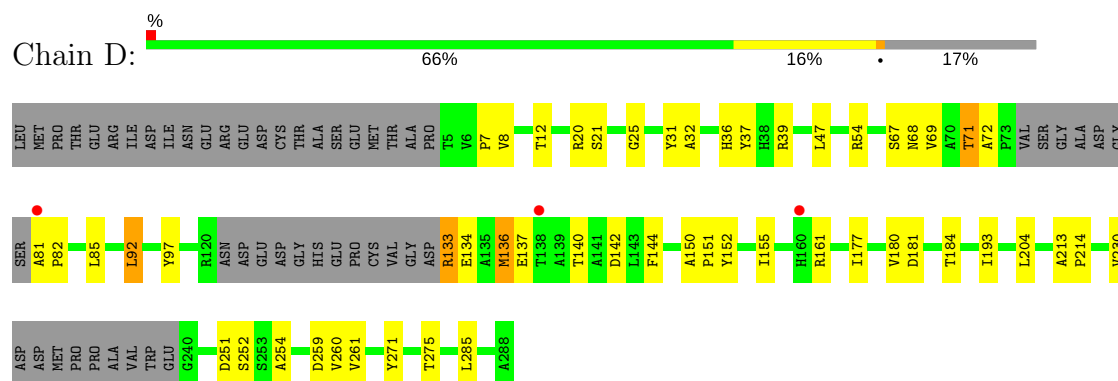


#### • Molecule 1: PTERIDINE REDUCTASE

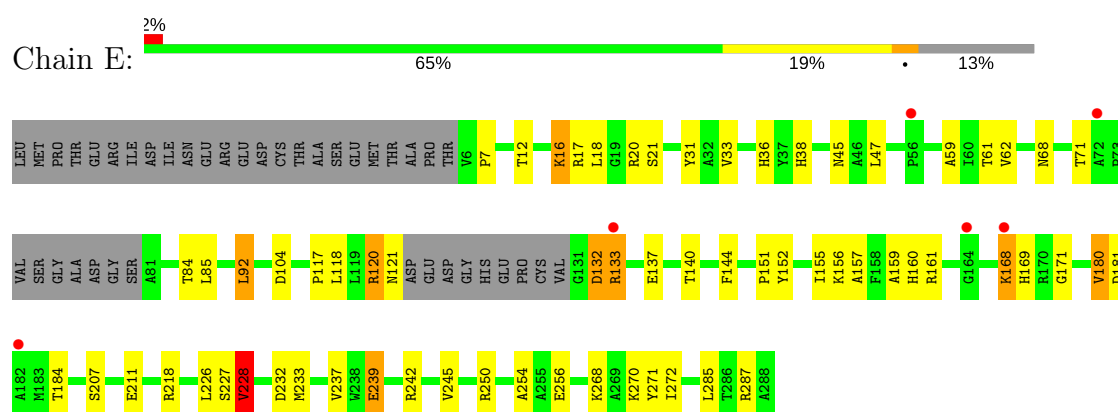




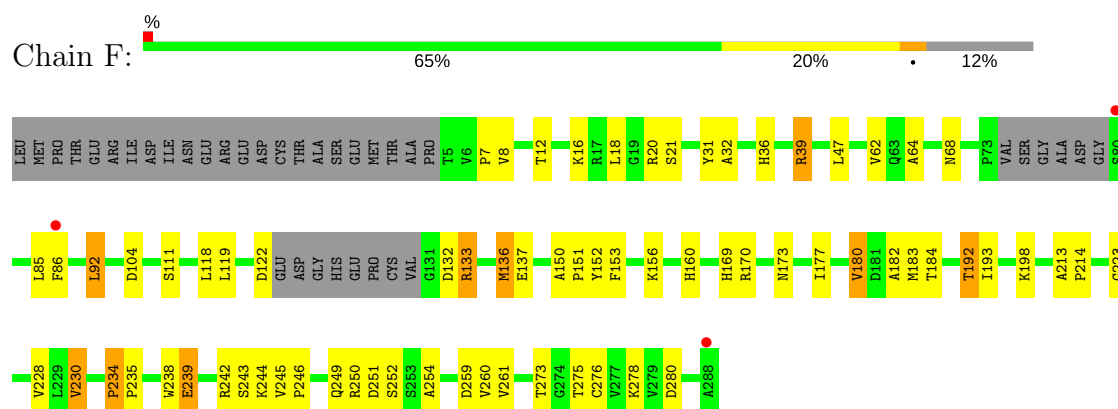
- Molecule 1: PTERIDINE REDUCTASE



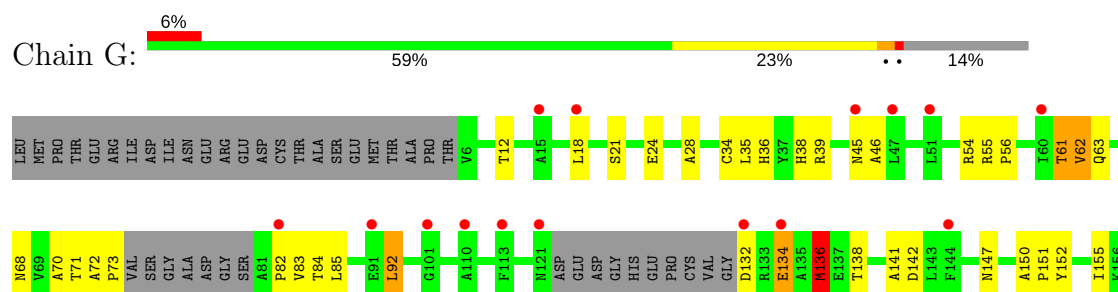
- Molecule 1: PTERIDINE REDUCTASE

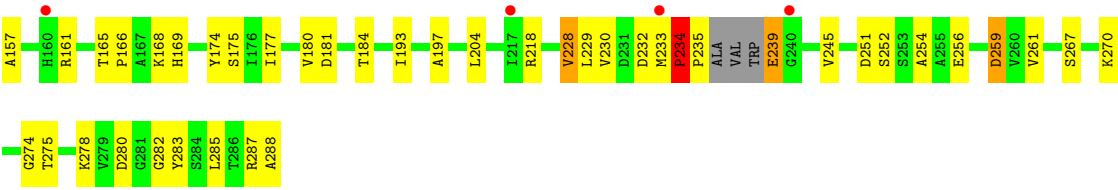


- Molecule 1: PTERIDINE REDUCTASE

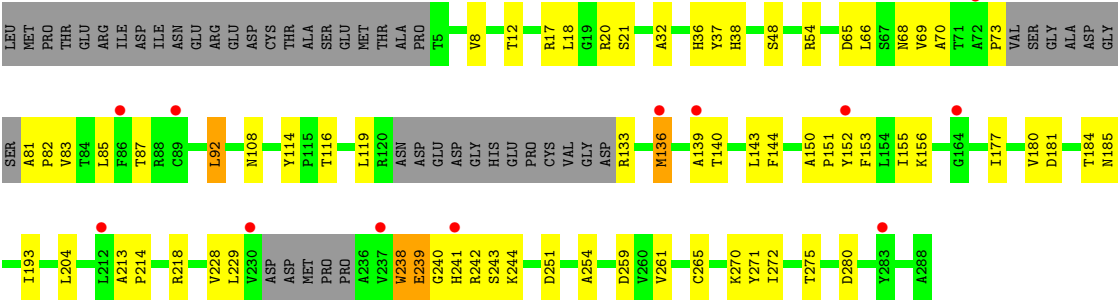


- Molecule 1: PTERIDINE REDUCTASE





● Molecule 1: PTERIDINE REDUCTASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.85Å 102.94Å 146.71Å 90.00° 108.32° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 29.82 – 2.60	Depositor EDS
% Data completeness (in resolution range)	91.0 (30.00-2.60) 87.3 (29.82-2.60)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.85 (at 2.61Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.267 , 0.337 0.273 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	18.8	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 19.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.166 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	17458	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 55.25 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.2472e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: NAP, TAQ

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	0.57	0/2081	0.79	3/2837 (0.1%)
1	B	0.57	0/2071	0.75	3/2822 (0.1%)
1	C	0.50	0/1988	0.74	4/2703 (0.1%)
1	D	0.51	0/1940	0.71	2/2638 (0.1%)
1	E	0.59	0/2031	0.77	5/2766 (0.2%)
1	F	0.63	1/2052 (0.0%)	0.82	6/2795 (0.2%)
1	G	0.59	0/1998	0.76	4/2718 (0.1%)
1	H	0.60	0/1977	0.73	3/2690 (0.1%)
All	All	0.57	1/16138 (0.0%)	0.76	30/21969 (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	B	0	2
1	D	0	1
1	G	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	192	THR	CB-CG2	-11.50	1.14	1.52

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	192	THR	OG1-CB-CG2	-12.69	80.81	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	259	ASP	CB-CG-OD2	7.54	125.08	118.30
1	H	251	ASP	CB-CG-OD2	6.45	124.11	118.30
1	G	251	ASP	CB-CG-OD2	6.29	123.97	118.30
1	A	122	ASP	CB-CG-OD2	6.20	123.88	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	131	GLY	Peptide
1	B	132	ASP	Peptide
1	D	81	ALA	Peptide
1	G	234	PRO	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	2041	0	2033	55	0
1	B	2031	0	2032	67	0
1	C	1954	0	1968	40	0
1	D	1906	0	1928	39	0
1	E	1992	0	1996	54	0
1	F	2013	0	2011	62	0
1	G	1962	0	1968	71	0
1	H	1941	0	1958	59	0
2	A	48	0	25	1	0
2	B	48	0	25	0	0
2	C	48	0	25	1	0
2	D	48	0	25	1	0
2	E	48	0	25	1	0
2	F	48	0	25	0	0
2	G	48	0	25	3	0
2	H	48	0	25	1	0
3	A	26	0	18	2	0
3	B	13	0	9	0	0
3	C	13	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	13	0	9	0	0
3	E	13	0	9	1	0
3	F	13	0	9	1	0
3	G	13	0	9	3	0
3	H	13	0	9	1	0
4	A	214	0	0	19	2
4	B	216	0	0	27	1
4	C	117	0	0	6	1
4	D	97	0	0	8	0
4	E	127	0	0	8	1
4	F	104	0	0	21	1
4	G	143	0	0	27	0
4	H	99	0	0	23	0
All	All	17458	0	16175	404	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 404 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:242:ARG:HH11	1:B:242:ARG:HG2	1.09	1.13
1:G:234:PRO:HB2	1:G:235:PRO:CD	1.78	1.11
1:C:81:ALA:HB1	1:C:82:PRO:HD2	1.22	1.10
1:F:180:VAL:HG13	4:F:2058:HOH:O	1.55	1.04
1:G:234:PRO:CB	1:G:235:PRO:HD3	1.88	1.03

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:2016:HOH:O	4:E:2018:HOH:O[2_646]	1.95	0.25
4:A:2174:HOH:O	4:F:2018:HOH:O[2_546]	2.11	0.09
4:A:2051:HOH:O	4:C:2023:HOH:O[2_545]	2.13	0.07

## 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	272/307 (89%)	253 (93%)	15 (6%)	4 (2%)	12	24
1	B	270/307 (88%)	240 (89%)	24 (9%)	6 (2%)	8	14
1	C	256/307 (83%)	234 (91%)	17 (7%)	5 (2%)	9	17
1	D	248/307 (81%)	231 (93%)	16 (6%)	1 (0%)	38	63
1	E	261/307 (85%)	239 (92%)	20 (8%)	2 (1%)	22	44
1	F	264/307 (86%)	243 (92%)	17 (6%)	4 (2%)	12	24
1	G	255/307 (83%)	235 (92%)	15 (6%)	5 (2%)	9	17
1	H	252/307 (82%)	233 (92%)	15 (6%)	4 (2%)	11	23
All	All	2078/2456 (85%)	1908 (92%)	139 (7%)	31 (2%)	12	24

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	ALA
1	B	74	VAL
1	B	75	SER
1	B	80	SER
1	B	81	ALA

### 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	212/241 (88%)	201 (95%)	11 (5%)	27	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	211/241 (88%)	201 (95%)	10 (5%)	30	57
1	C	203/241 (84%)	196 (97%)	7 (3%)	42	69
1	D	198/241 (82%)	190 (96%)	8 (4%)	36	64
1	E	207/241 (86%)	196 (95%)	11 (5%)	26	50
1	F	210/241 (87%)	198 (94%)	12 (6%)	24	47
1	G	205/241 (85%)	196 (96%)	9 (4%)	33	60
1	H	201/241 (83%)	195 (97%)	6 (3%)	46	74
All	All	1647/1928 (85%)	1573 (96%)	74 (4%)	32	59

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	137	GLU
1	E	133	ARG
1	H	54	ARG
1	D	230	VAL
1	E	71	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	216	GLN
1	D	216	GLN
1	F	216	GLN
1	C	160	HIS
1	E	216	GLN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

17 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	NAP	A	300	-	44,52,52	1.58	4 (9%)	51,80,80	1.79	4 (7%)
3	TAQ	A	301	-	14,14,14	1.86	3 (21%)	19,20,20	1.94	4 (21%)
3	TAQ	A	302	-	14,14,14	1.92	1 (7%)	19,20,20	2.37	6 (31%)
2	NAP	B	300	-	44,52,52	1.51	3 (6%)	51,80,80	1.73	4 (7%)
3	TAQ	B	301	-	14,14,14	1.68	2 (14%)	19,20,20	2.18	5 (26%)
2	NAP	C	300	-	44,52,52	1.49	3 (6%)	51,80,80	1.71	4 (7%)
3	TAQ	C	301	-	14,14,14	1.97	1 (7%)	19,20,20	2.06	4 (21%)
2	NAP	D	300	-	44,52,52	1.59	3 (6%)	51,80,80	1.82	6 (11%)
3	TAQ	D	301	-	14,14,14	1.42	1 (7%)	19,20,20	2.25	4 (21%)
2	NAP	E	300	-	44,52,52	1.61	4 (9%)	51,80,80	1.76	6 (11%)
3	TAQ	E	301	-	14,14,14	1.63	1 (7%)	19,20,20	2.18	5 (26%)
2	NAP	F	300	-	44,52,52	1.60	3 (6%)	51,80,80	1.72	3 (5%)
3	TAQ	F	301	-	14,14,14	1.56	2 (14%)	19,20,20	2.06	5 (26%)
2	NAP	G	300	-	44,52,52	1.62	4 (9%)	51,80,80	1.80	5 (9%)
3	TAQ	G	301	-	14,14,14	1.28	2 (14%)	19,20,20	1.92	4 (21%)
2	NAP	H	300	-	44,52,52	1.58	4 (9%)	51,80,80	1.95	3 (5%)
3	TAQ	H	301	-	14,14,14	1.68	1 (7%)	19,20,20	1.95	4 (21%)

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	NAP	A	300	-	-	0/27/67/67	0/5/5/5
3	TAQ	A	301	-	-	0/0/0/0	0/2/2/2
3	TAQ	A	302	-	-	0/0/0/0	0/2/2/2
2	NAP	B	300	-	-	0/27/67/67	0/5/5/5
3	TAQ	B	301	-	-	0/0/0/0	0/2/2/2
2	NAP	C	300	-	-	0/27/67/67	0/5/5/5
3	TAQ	C	301	-	-	0/0/0/0	0/2/2/2
2	NAP	D	300	-	-	0/27/67/67	0/5/5/5
3	TAQ	D	301	-	-	0/0/0/0	0/2/2/2
2	NAP	E	300	-	-	0/27/67/67	0/5/5/5
3	TAQ	E	301	-	-	0/0/0/0	0/2/2/2
2	NAP	F	300	-	-	0/27/67/67	0/5/5/5
3	TAQ	F	301	-	-	0/0/0/0	0/2/2/2
2	NAP	G	300	-	-	0/27/67/67	0/5/5/5
3	TAQ	G	301	-	-	0/0/0/0	0/2/2/2
2	NAP	H	300	-	-	0/27/67/67	0/5/5/5
3	TAQ	H	301	-	-	0/0/0/0	0/2/2/2

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	TAQ	C7-C4	-6.59	1.39	1.45
3	A	302	TAQ	C7-C4	-6.13	1.40	1.45
3	A	301	TAQ	C7-C4	-5.58	1.40	1.45
3	H	301	TAQ	C7-C4	-5.48	1.40	1.45
3	E	301	TAQ	C7-C4	-5.01	1.41	1.45

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	300	NAP	N3A-C2A-N1A	-11.42	118.91	128.86
2	D	300	NAP	N3A-C2A-N1A	-10.74	119.50	128.86
2	G	300	NAP	N3A-C2A-N1A	-10.60	119.63	128.86
2	A	300	NAP	N3A-C2A-N1A	-10.57	119.66	128.86
2	B	300	NAP	N3A-C2A-N1A	-10.15	120.02	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	NAP	1	0
3	A	301	TAQ	1	0
3	A	302	TAQ	1	0
2	C	300	NAP	1	0
2	D	300	NAP	1	0
2	E	300	NAP	1	0
3	E	301	TAQ	1	0
3	F	301	TAQ	1	0
2	G	300	NAP	3	0
3	G	301	TAQ	3	0
2	H	300	NAP	1	0
3	H	301	TAQ	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	276/307 (89%)	0.00	4 (1%) 75 71	4, 18, 35, 46	1 (0%)
1	B	274/307 (89%)	-0.01	3 (1%) 80 77	6, 18, 34, 46	1 (0%)
1	C	264/307 (85%)	-0.17	2 (0%) 86 83	5, 19, 43, 55	5 (1%)
1	D	256/307 (83%)	-0.20	3 (1%) 79 75	9, 18, 35, 56	2 (0%)
1	E	267/307 (86%)	0.19	6 (2%) 62 56	9, 19, 31, 42	0
1	F	270/307 (87%)	0.03	3 (1%) 80 77	9, 19, 32, 50	1 (0%)
1	G	263/307 (85%)	0.69	19 (7%) 16 12	9, 19, 47, 67	5 (1%)
1	H	260/307 (84%)	0.47	12 (4%) 33 26	10, 19, 41, 72	2 (0%)
All	All	2130/2456 (86%)	0.12	52 (2%) 59 52	4, 19, 38, 72	17 (0%)

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	121	ASN	4.2
1	A	122	ASP	4.2
1	F	80	SER	3.9
1	H	237	VAL	3.6
1	H	72	ALA	3.2

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

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

### 6.3 Carbohydrates [i](#)

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	TAQ	B	301	13/13	0.96	0.17	1.70	13,14,15,15	0
3	TAQ	F	301	13/13	0.93	0.19	0.60	13,14,15,15	0
3	TAQ	C	301	13/13	0.96	0.15	0.48	12,14,15,16	0
2	NAP	A	300	48/48	0.96	0.17	0.38	8,15,18,21	0
3	TAQ	G	301	13/13	0.81	0.26	0.33	13,14,15,16	0
3	TAQ	A	301	13/13	0.97	0.17	0.10	13,14,15,15	0
3	TAQ	E	301	13/13	0.94	0.17	0.10	12,14,15,15	0
2	NAP	H	300	48/48	0.91	0.19	0.03	9,15,19,21	0
2	NAP	B	300	48/48	0.96	0.17	-0.03	9,15,18,21	0
2	NAP	F	300	48/48	0.96	0.15	-0.30	9,15,18,21	0
2	NAP	G	300	48/48	0.91	0.18	-0.74	9,15,19,21	0
2	NAP	C	300	48/48	0.98	0.13	-0.85	9,15,19,21	0
2	NAP	D	300	48/48	0.96	0.14	-0.89	9,15,19,21	0
2	NAP	E	300	48/48	0.96	0.14	-0.96	9,15,19,22	0
3	TAQ	H	301	13/13	0.91	0.18	-1.07	13,14,15,15	0
3	TAQ	D	301	13/13	0.96	0.12	-1.14	13,14,15,16	0
3	TAQ	A	302	13/13	0.86	0.17	-	25,28,31,31	0

## 6.5 Other polymers

There are no such residues in this entry.