



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 04:46 AM GMT

PDB ID : 2YW9  
Title : Crystal structure of TT0143 from *Thermus thermophilus* HB8  
Authors : Miyano, M.; Ago, H.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2007-04-20  
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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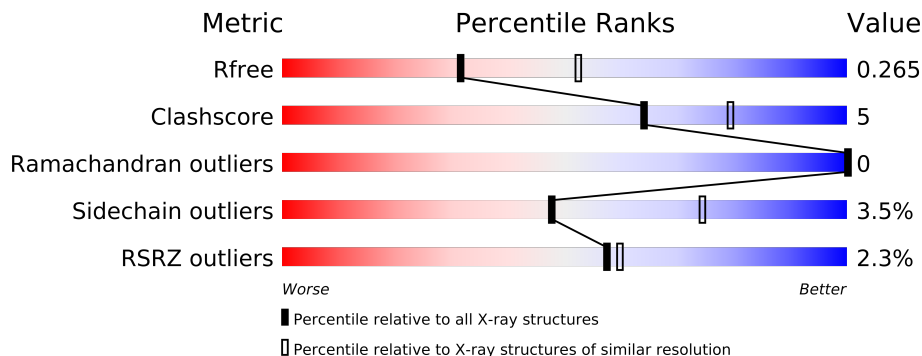
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	261	
1	B	261	
1	C	261	
1	D	261	
1	E	261	
1	F	261	
1	G	261	
1	H	261	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14777 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Enoyl-[acyl carrier protein] reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	1	0
			1767	1134	298	330	5			
1	B	255	Total	C	N	O	S	0	1	0
			1846	1192	309	339	6			
1	C	245	Total	C	N	O	S	0	1	0
			1775	1145	298	326	6			
1	D	247	Total	C	N	O	S	0	1	0
			1777	1143	295	334	5			
1	E	246	Total	C	N	O	S	0	0	0
			1767	1136	295	329	7			
1	F	242	Total	C	N	O	S	0	1	0
			1749	1126	298	320	5			
1	G	255	Total	C	N	O	S	0	1	0
			1861	1197	313	346	5			
1	H	246	Total	C	N	O	S	0	0	0
			1753	1126	295	327	5			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (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	D	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 water.

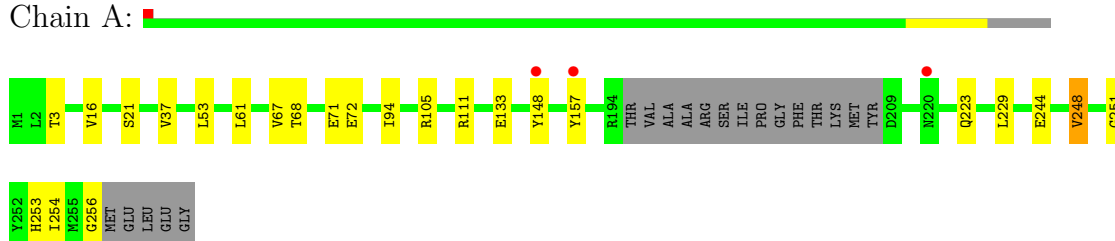
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	45	Total	O	0	0
			45	45		
3	B	53	Total	O	0	0
			53	53		
3	C	47	Total	O	0	0
			47	47		
3	D	44	Total	O	0	0
			44	44		
3	E	38	Total	O	0	0
			38	38		
3	F	39	Total	O	0	0
			39	39		
3	G	61	Total	O	0	0
			61	61		
3	H	59	Total	O	0	0
			59	59		

### 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.

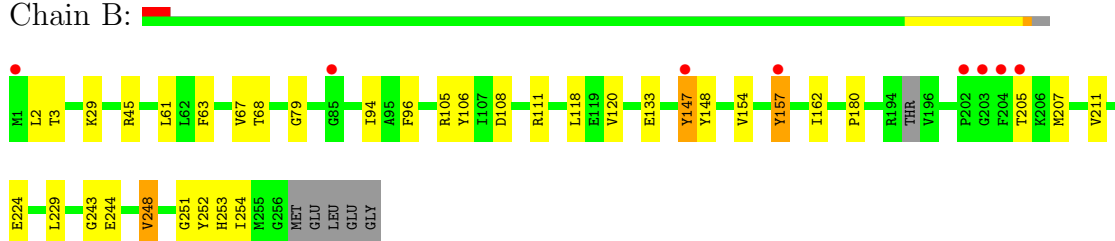
- Molecule 1: Enoyl-[acyl carrier protein] reductase

Chain A:



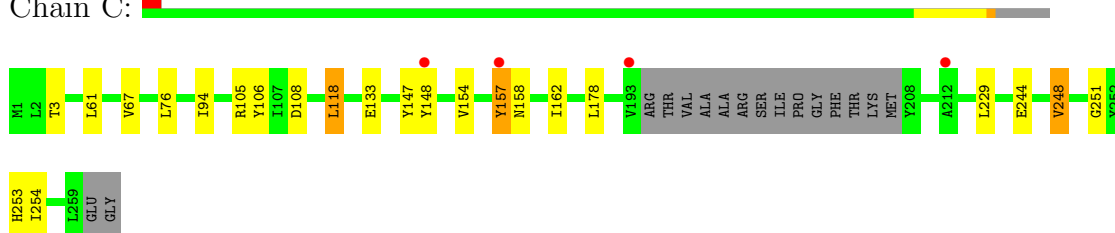
- Molecule 1: Enoyl-[acyl carrier protein] reductase

Chain B:



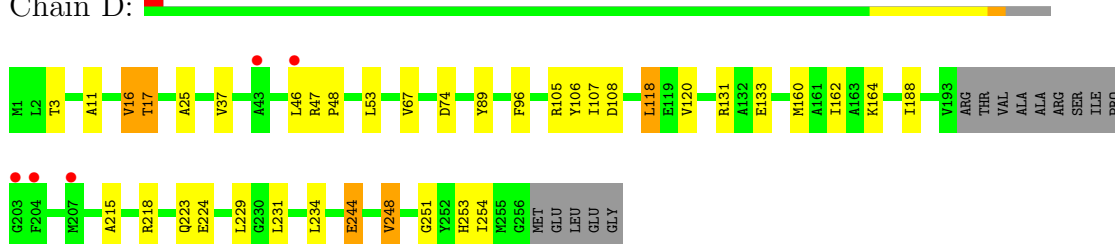
- Molecule 1: Enoyl-[acyl carrier protein] reductase

Chain C:

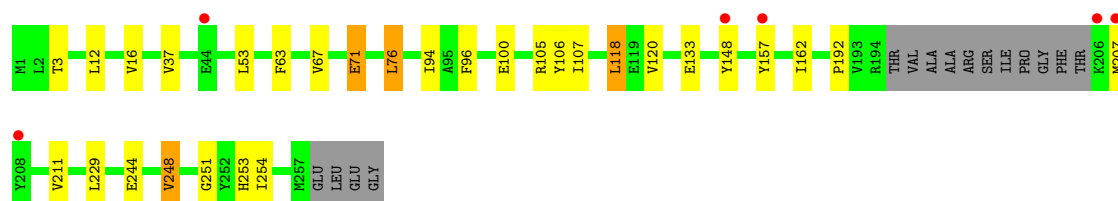


- Molecule 1: Enoyl-[acyl carrier protein] reductase

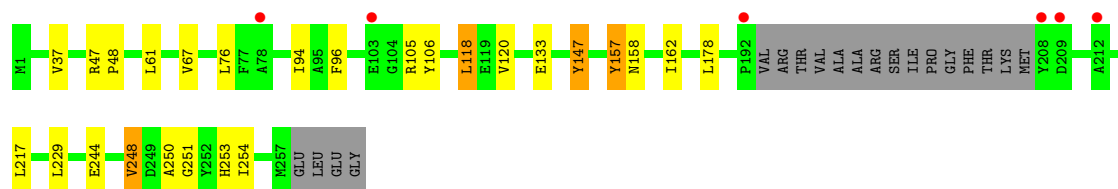
Chain D:



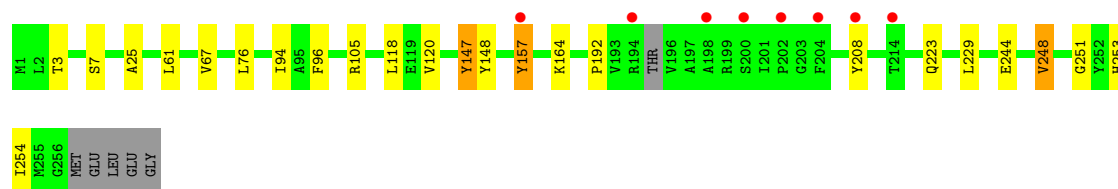
- Molecule 1: Enoyl-[acyl carrier protein] reductase

Chain E: 

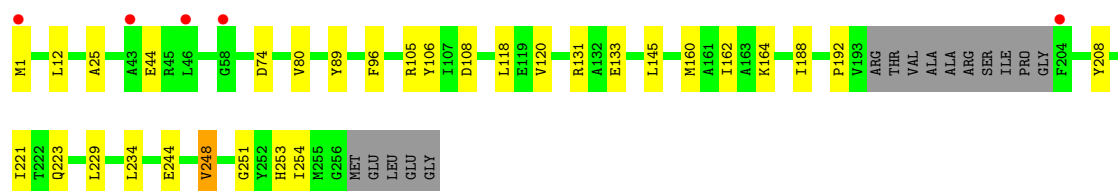
- Molecule 1: Enoyl-[acyl carrier protein] reductase

Chain F: 

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

Chain G: 

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

Chain H: 

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.09Å 107.13Å 184.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 37.88 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.50) 100.0 (37.88-2.50)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.03 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.3.0027	Depositor
R, $R_{free}$	0.222 , 0.263 0.224 , 0.265	Depositor DCC
$R_{free}$ test set	6750 reflections (11.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.8	Xtriage
Anisotropy	0.817	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 18.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	16 of 66626 reflections (0.024%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14777	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	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 42.97 % 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 1.8889e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.39	2/1797 (0.1%)	0.50	0/2443
1	B	0.36	0/1880	0.51	0/2559
1	C	0.32	0/1806	0.48	0/2457
1	D	0.33	0/1808	0.50	0/2463
1	E	0.31	0/1795	0.48	0/2445
1	F	0.32	0/1781	0.48	0/2425
1	G	0.34	0/1895	0.50	0/2578
1	H	0.34	0/1781	0.51	0/2428
All	All	0.34	2/14543 (0.0%)	0.49	0/19798

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	148	TYR	CE2-CZ	-5.70	1.31	1.38
1	A	148	TYR	CG-CD1	-5.21	1.32	1.39

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1767	0	1765	17	0
1	B	1846	0	1829	32	0
1	C	1775	0	1767	21	0
1	D	1777	0	1740	32	0
1	E	1767	0	1737	24	0
1	F	1749	0	1723	20	0
1	G	1861	0	1840	18	0
1	H	1753	0	1699	18	0
2	D	48	0	25	4	0
2	H	48	0	25	2	0
3	A	45	0	0	1	0
3	B	53	0	0	1	0
3	C	47	0	0	1	0
3	D	44	0	0	1	0
3	E	38	0	0	2	0
3	F	39	0	0	1	0
3	G	61	0	0	0	0
3	H	59	0	0	1	0
All	All	14777	0	14150	155	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (155) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:253:HIS:HE1	1:D:244[B]:GLU:OE2	1.51	0.94
1:C:147[B]:TYR:CE2	1:C:157:TYR:CE2	2.72	0.77
1:B:253:HIS:CE1	1:D:244[B]:GLU:OE2	2.37	0.77
1:F:147[A]:TYR:CE2	1:F:157:TYR:CE2	2.73	0.76
1:B:147[A]:TYR:CE1	1:B:157:TYR:CE2	2.76	0.73
1:C:147[B]:TYR:CZ	1:C:157:TYR:HE2	2.06	0.72
1:G:147[A]:TYR:CE2	1:G:157:TYR:CE2	2.78	0.71
1:G:147[A]:TYR:CZ	1:G:157:TYR:HE2	2.08	0.71
1:H:229:LEU:HD22	1:H:248:VAL:HG22	1.73	0.70
1:D:229:LEU:HD22	1:D:248:VAL:HG22	1.73	0.70
1:B:244:GLU:OE2	1:D:253:HIS:HE1	1.74	0.70
1:F:147[A]:TYR:CZ	1:F:157:TYR:HE2	2.11	0.69
1:E:71:GLU:OE2	3:E:280:HOH:O	2.13	0.66
1:E:67:VAL:HG11	1:E:94:ILE:HD13	1.78	0.65
1:E:244:GLU:OE2	1:G:253:HIS:HE1	1.80	0.64
1:C:158:ASN:HB3	3:C:263:HOH:O	1.98	0.64
1:F:147[A]:TYR:CE2	1:F:157:TYR:HE2	2.14	0.63
1:G:67:VAL:HG11	1:G:94:ILE:HD13	1.82	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:105:ARG:NH2	1:H:133:GLU:OE1	2.28	0.62
1:H:25:ALA:HB2	1:H:223:GLN:HG2	1.82	0.61
1:G:147[A]:TYR:CE2	1:G:157:TYR:HE2	2.17	0.60
1:B:244:GLU:OE1	3:B:263:HOH:O	2.16	0.60
1:A:133:GLU:OE1	1:B:105:ARG:NH2	2.33	0.60
1:B:147[A]:TYR:CE1	1:B:157:TYR:HE2	2.19	0.59
1:F:67:VAL:HG11	1:F:94:ILE:HD13	1.85	0.59
1:C:67:VAL:HG11	1:C:94:ILE:HD13	1.85	0.58
1:F:244:GLU:OE2	1:H:253:HIS:HE1	1.87	0.58
1:D:25:ALA:HB2	1:D:223:GLN:HG2	1.83	0.58
1:C:147[B]:TYR:CZ	1:C:157:TYR:CE2	2.89	0.57
1:A:229:LEU:CD2	1:A:248:VAL:HG22	2.34	0.57
1:E:3:THR:HG22	1:G:3:THR:HG22	1.85	0.57
1:B:147[B]:TYR:OH	1:B:207:MET:HG2	2.04	0.57
1:E:229:LEU:CD2	1:E:248:VAL:HG22	2.35	0.57
1:F:253:HIS:HE1	1:H:244:GLU:OE1	1.89	0.56
1:E:251:GLY:O	1:E:254:ILE:HG12	2.06	0.56
1:G:25:ALA:HB2	1:G:223:GLN:HG2	1.86	0.56
1:A:67:VAL:HG11	1:A:94:ILE:HD13	1.87	0.56
1:B:67:VAL:HG11	1:B:94:ILE:HD13	1.88	0.55
1:A:133:GLU:CD	1:B:105:ARG:HH22	2.09	0.55
1:D:251:GLY:O	1:D:254:ILE:HG12	2.07	0.55
1:B:3:THR:HG22	1:D:3:THR:HG22	1.89	0.55
1:B:147[A]:TYR:CZ	1:B:157:TYR:HE2	2.24	0.54
1:B:243:GLY:HA3	1:D:254:ILE:HD13	1.89	0.54
1:A:256:GLY:C	3:A:285:HOH:O	2.46	0.54
1:A:253:HIS:HE1	1:C:244:GLU:OE2	1.91	0.54
1:H:223:GLN:NE2	3:H:510:HOH:O	2.41	0.53
1:D:47:ARG:HB3	1:D:48:PRO:HD3	1.89	0.53
1:C:105:ARG:NH2	1:D:133:GLU:OE1	2.33	0.52
1:H:105:ARG:HD3	1:H:108:ASP:OD2	2.09	0.52
1:H:192:PRO:HB2	1:H:208:TYR:HD1	1.75	0.52
1:A:244:GLU:OE2	1:C:253:HIS:HE1	1.92	0.51
1:A:3:THR:HG22	1:C:3:THR:HG22	1.92	0.51
1:A:71:GLU:HG2	1:A:72:GLU:N	2.26	0.51
1:H:251:GLY:O	1:H:254:ILE:HG12	2.11	0.51
1:B:244:GLU:OE2	1:D:253:HIS:CE1	2.61	0.51
1:A:68:THR:HA	1:B:111:ARG:NH1	2.26	0.51
1:G:229:LEU:CD2	1:G:248:VAL:HG22	2.41	0.51
1:F:147[A]:TYR:CZ	1:F:157:TYR:CE2	2.95	0.51
1:D:160:MET:CE	1:D:164:LYS:HE2	2.41	0.51
1:B:229:LEU:CD2	1:B:248:VAL:HG22	2.41	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:74:ASP:OD1	1:H:131:ARG:NH1	2.44	0.50
1:C:133:GLU:OE1	1:D:105:ARG:NH2	2.43	0.50
1:G:147[A]:TYR:CZ	1:G:157:TYR:CE2	2.94	0.50
1:A:229:LEU:HD22	1:A:248:VAL:HG22	1.93	0.50
1:B:2:LEU:HD23	1:D:231:LEU:CD2	2.41	0.50
1:F:229:LEU:CD2	1:F:248:VAL:HG22	2.41	0.50
1:D:74:ASP:OD1	1:D:131:ARG:NH1	2.45	0.50
1:D:188:ILE:HG23	1:D:229:LEU:HD23	1.93	0.50
1:A:21:SER:O	1:A:223:GLN:NE2	2.39	0.49
1:B:229:LEU:HD23	1:B:248:VAL:HG22	1.93	0.49
1:H:188:ILE:HG23	1:H:229:LEU:HD23	1.93	0.49
1:H:96:PHE:HB3	1:H:120:VAL:HG11	1.94	0.49
1:C:229:LEU:CD2	1:C:248:VAL:HG22	2.43	0.49
1:E:253:HIS:HE1	1:G:244:GLU:OE2	1.96	0.48
1:A:105:ARG:NH2	1:B:133:GLU:OE1	2.43	0.48
2:D:500:NAP:H2N	2:D:500:NAP:O1N	2.12	0.48
1:G:251:GLY:O	1:G:254:ILE:HG12	2.14	0.48
1:A:251:GLY:O	1:A:254:ILE:HG12	2.14	0.48
2:H:501:NAP:O1N	2:H:501:NAP:H2N	2.14	0.47
1:A:16:VAL:HG12	1:A:53:LEU:HD13	1.96	0.47
1:E:105:ARG:NH2	1:F:133:GLU:OE1	2.35	0.47
1:D:105:ARG:HD3	1:D:108:ASP:OD2	2.13	0.47
1:B:105:ARG:HD3	1:B:108:ASP:OD2	2.15	0.46
1:H:229:LEU:CD2	1:H:248:VAL:HG22	2.44	0.46
1:E:244:GLU:OE2	1:G:253:HIS:CE1	2.65	0.46
1:G:148:TYR:CE1	1:G:253:HIS:HB2	2.50	0.46
1:B:211:VAL:HG22	1:B:252:TYR:CG	2.51	0.46
1:B:148:TYR:CE1	1:B:253:HIS:HB2	2.50	0.46
1:C:105:ARG:HD3	1:C:108:ASP:OD2	2.16	0.46
1:D:160:MET:HE1	1:D:164:LYS:HE2	1.97	0.46
1:E:229:LEU:HD23	1:E:248:VAL:HG22	1.98	0.46
1:C:148:TYR:CE1	1:C:253:HIS:HB2	2.51	0.45
1:B:180:PRO:HG3	1:D:218:ARG:NH1	2.32	0.45
1:E:229:LEU:HD22	1:E:248:VAL:HG22	1.99	0.45
1:A:111:ARG:NH1	1:B:68:THR:HA	2.32	0.45
1:E:133:GLU:OE1	1:F:105:ARG:NH2	2.44	0.44
1:F:96:PHE:HB3	1:F:120:VAL:HG11	1.99	0.44
1:E:192:PRO:HG2	1:E:211:VAL:HG21	1.99	0.44
1:D:17:THR:HG21	2:D:500:NAP:O1X	2.17	0.44
1:D:17:THR:HG22	1:D:46:LEU:HD13	1.98	0.44
1:D:17:THR:HG22	1:D:46:LEU:HD22	1.99	0.44
1:D:106:TYR:CE2	1:D:162:ILE:HG13	2.52	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:16:VAL:HG12	1:E:53:LEU:HD13	1.99	0.44
1:D:89:TYR:HB3	1:D:234:LEU:HD22	2.00	0.44
1:E:118:LEU:HD22	1:F:118:LEU:HD22	2.00	0.44
1:D:215:ALA:O	1:D:218:ARG:HD3	2.18	0.44
1:D:11:ALA:HB3	1:D:37:VAL:HG12	2.00	0.43
1:H:160:MET:CE	1:H:164:LYS:HE2	2.48	0.43
1:D:16:VAL:HG13	1:D:53:LEU:CD1	2.48	0.43
1:H:106:TYR:CE2	1:H:162:ILE:HG13	2.53	0.43
1:B:106:TYR:CE2	1:B:162:ILE:HG13	2.53	0.43
1:D:224:GLU:HB2	3:D:538:HOH:O	2.19	0.43
1:E:100:GLU:O	3:E:291:HOH:O	2.21	0.43
1:B:106:TYR:CZ	1:B:162:ILE:HG13	2.54	0.43
1:G:96:PHE:HB3	1:G:120:VAL:HG11	2.01	0.43
1:D:67:VAL:HG22	2:D:500:NAP:N1A	2.34	0.43
1:E:106:TYR:CZ	1:E:162:ILE:HG13	2.54	0.43
1:B:154:VAL:O	1:B:157:TYR:HB2	2.19	0.43
1:G:147[A]:TYR:CE2	1:G:164:LYS:HG3	2.54	0.43
1:E:148:TYR:CD1	1:E:253:HIS:HB2	2.54	0.43
1:B:251:GLY:O	1:B:254:ILE:HG12	2.18	0.43
1:B:63:PHE:HE1	1:B:79:GLY:HA3	1.83	0.43
1:F:158:ASN:HB3	3:F:271:HOH:O	2.19	0.42
2:D:500:NAP:N7N	2:D:500:NAP:O1N	2.47	0.42
1:D:96:PHE:HB3	1:D:120:VAL:HG11	2.00	0.42
1:C:251:GLY:O	1:C:254:ILE:HG12	2.20	0.42
1:G:229:LEU:HD23	1:G:248:VAL:HG22	2.02	0.42
1:C:147[B]:TYR:CE2	1:C:157:TYR:HE2	2.21	0.42
1:A:61:LEU:HA	1:A:61:LEU:HD12	1.89	0.42
1:F:251:GLY:O	1:F:254:ILE:HG12	2.19	0.42
1:H:89:TYR:HB3	1:H:234:LEU:HD22	2.01	0.42
1:G:192:PRO:HB2	1:G:208:TYR:HD1	1.84	0.42
1:F:47:ARG:HB3	1:F:48:PRO:HD3	2.01	0.42
1:H:221:ILE:HD13	1:H:248:VAL:O	2.20	0.42
1:F:229:LEU:HD22	1:F:248:VAL:HG22	2.02	0.42
2:H:501:NAP:O1N	2:H:501:NAP:N7N	2.52	0.42
1:E:63:PHE:HB3	1:E:76:LEU:HD12	2.01	0.42
1:E:12:LEU:HD21	1:E:76:LEU:HD21	2.02	0.42
1:E:96:PHE:HB3	1:E:120:VAL:HG11	2.03	0.41
1:F:106:TYR:CE2	1:F:162:ILE:HG13	2.55	0.41
1:C:148:TYR:CD1	1:C:253:HIS:HB2	2.56	0.41
1:C:178:LEU:HD21	1:D:107:ILE:HD13	2.03	0.41
1:B:96:PHE:HB3	1:B:120:VAL:HG11	2.03	0.41
1:E:107:ILE:HD13	1:F:178:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:63:PHE:CB	1:E:76:LEU:HD12	2.51	0.41
1:F:217:LEU:HB2	1:F:250:ALA:HB1	2.02	0.41
1:H:12:LEU:HD22	1:H:80:VAL:HG21	2.03	0.41
1:C:229:LEU:HD23	1:C:248:VAL:HG22	2.03	0.40
1:C:154:VAL:O	1:C:157:TYR:HB2	2.21	0.40
1:B:147[A]:TYR:CZ	1:B:157:TYR:CE2	3.05	0.40
1:E:229:LEU:HD23	1:E:248:VAL:CG2	2.51	0.40
1:C:118:LEU:CD2	1:D:118:LEU:HD22	2.50	0.40
1:C:106:TYR:CE2	1:C:162:ILE:HG13	2.56	0.40
1:F:106:TYR:CZ	1:F:162:ILE:HG13	2.57	0.40
1:B:29:LYS:HZ3	1:B:224:GLU:HG3	1.86	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	239/261 (92%)	236 (99%)	3 (1%)	0	100	100
1	B	252/261 (97%)	250 (99%)	2 (1%)	0	100	100
1	C	242/261 (93%)	238 (98%)	4 (2%)	0	100	100
1	D	244/261 (94%)	237 (97%)	7 (3%)	0	100	100
1	E	242/261 (93%)	239 (99%)	3 (1%)	0	100	100
1	F	239/261 (92%)	237 (99%)	2 (1%)	0	100	100
1	G	252/261 (97%)	250 (99%)	2 (1%)	0	100	100
1	H	242/261 (93%)	233 (96%)	9 (4%)	0	100	100
All	All	1952/2088 (94%)	1920 (98%)	32 (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	167/197 (85%)	164 (98%)	3 (2%)	71	91
1	B	170/197 (86%)	162 (95%)	8 (5%)	36	61
1	C	164/197 (83%)	159 (97%)	5 (3%)	53	80
1	D	163/197 (83%)	157 (96%)	6 (4%)	45	72
1	E	163/197 (83%)	156 (96%)	7 (4%)	40	65
1	F	159/197 (81%)	151 (95%)	8 (5%)	34	58
1	G	173/197 (88%)	165 (95%)	8 (5%)	37	62
1	H	158/197 (80%)	153 (97%)	5 (3%)	51	77
All	All	1317/1576 (84%)	1267 (96%)	50 (4%)	48	71

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
1	A	157	TYR
1	A	248	VAL
1	B	45	ARG
1	B	61	LEU
1	B	118	LEU
1	B	147[A]	TYR
1	B	147[B]	TYR
1	B	157	TYR
1	B	205	THR
1	B	248	VAL
1	C	61	LEU
1	C	76	LEU
1	C	118	LEU
1	C	157	TYR
1	C	248	VAL
1	D	16	VAL
1	D	17	THR
1	D	118	LEU
1	D	244[A]	GLU
1	D	244[B]	GLU

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Mol	Chain	Res	Type
1	D	248	VAL
1	E	37	VAL
1	E	71	GLU
1	E	76	LEU
1	E	118	LEU
1	E	157	TYR
1	E	207	MET
1	E	248	VAL
1	F	37	VAL
1	F	61	LEU
1	F	76	LEU
1	F	118	LEU
1	F	147[A]	TYR
1	F	147[B]	TYR
1	F	157	TYR
1	F	248	VAL
1	G	7	SER
1	G	61	LEU
1	G	76	LEU
1	G	118	LEU
1	G	147[A]	TYR
1	G	147[B]	TYR
1	G	157	TYR
1	G	248	VAL
1	H	1	MET
1	H	44	GLU
1	H	118	LEU
1	H	145	LEU
1	H	248	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	253	HIS
1	B	253	HIS
1	C	220	ASN
1	C	253	HIS
1	D	253	HIS
1	E	220	ASN
1	E	253	HIS
1	F	220	ASN

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Mol	Chain	Res	Type
1	F	253	HIS
1	G	223	GLN
1	G	253	HIS
1	H	112	GLN
1	H	220	ASN
1	H	223	GLN
1	H	253	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

2 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	D	500	-	52,52,52	1.32	3 (5%)	80,80,80	1.86	10 (12%)
2	NAP	H	501	-	52,52,52	1.33	3 (5%)	80,80,80	1.78	9 (11%)

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	D	500	-	-	0/35/67/67	0/3/5/5
2	NAP	H	501	-	-	0/35/67/67	0/3/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	501	NAP	O7N-C7N	7.28	1.41	1.24
2	D	500	NAP	O7N-C7N	7.19	1.41	1.24
2	H	501	NAP	C2A-N3A	3.29	1.38	1.32
2	D	500	NAP	C2A-N3A	3.19	1.38	1.32
2	H	501	NAP	C2A-N1A	2.33	1.38	1.33
2	D	500	NAP	C2A-N1A	2.17	1.38	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500	NAP	N3A-C2A-N1A	-10.58	119.87	128.71
2	H	501	NAP	N3A-C2A-N1A	-9.81	120.51	128.71
2	D	500	NAP	O4B-C1B-N9A	8.11	115.99	108.44
2	H	501	NAP	O4B-C1B-N9A	7.43	115.35	108.44
2	D	500	NAP	O4B-C1B-C2B	-4.58	102.67	106.95
2	H	501	NAP	O4B-C1B-C2B	-4.16	103.06	106.95
2	H	501	NAP	N3A-C4A-N9A	4.09	132.81	125.43
2	D	500	NAP	N3A-C4A-N9A	3.53	131.81	125.43
2	H	501	NAP	C5A-C4A-N3A	-2.51	120.23	125.70
2	D	500	NAP	P2B-O2B-C2B	-2.43	116.85	121.96
2	D	500	NAP	C5A-C4A-N3A	-2.37	120.54	125.70
2	D	500	NAP	C2A-N3A-C4A	2.29	120.52	114.01
2	D	500	NAP	O4D-C1D-N1N	2.27	110.28	107.95
2	D	500	NAP	C4A-C5A-N7A	-2.27	107.58	109.52
2	H	501	NAP	C2A-N3A-C4A	2.18	120.20	114.01
2	H	501	NAP	N7A-C8A-N9A	-2.17	108.22	114.36
2	D	500	NAP	N7A-C8A-N9A	-2.11	108.40	114.36
2	H	501	NAP	O4D-C1D-N1N	2.07	110.06	107.95
2	H	501	NAP	C4A-C5A-N7A	-2.03	107.79	109.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	242/261 (92%)	-0.09	3 (1%) 75 77	18, 31, 42, 55	0
1	B	255/261 (97%)	0.02	8 (3%) 47 48	18, 31, 52, 68	0
1	C	245/261 (93%)	-0.05	4 (1%) 68 71	18, 31, 43, 55	0
1	D	247/261 (94%)	-0.15	5 (2%) 62 64	18, 30, 47, 67	0
1	E	246/261 (94%)	-0.07	6 (2%) 56 58	18, 31, 43, 73	0
1	F	242/261 (92%)	-0.08	6 (2%) 54 57	18, 31, 42, 61	0
1	G	255/261 (97%)	-0.05	8 (3%) 47 48	18, 31, 53, 64	0
1	H	246/261 (94%)	-0.14	5 (2%) 62 64	18, 30, 45, 62	0
All	All	1978/2088 (94%)	-0.08	45 (2%) 57 60	18, 31, 45, 73	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	200	SER	5.1
1	B	202	PRO	4.6
1	F	208	TYR	4.6
1	H	204	PHE	4.1
1	H	43	ALA	3.9
1	D	203	GLY	3.9
1	D	43	ALA	3.4
1	E	157	TYR	3.3
1	A	148	TYR	3.2
1	E	208	TYR	3.1
1	B	204	PHE	3.1
1	H	46	LEU	2.9
1	D	204	PHE	2.9
1	B	203	GLY	2.9
1	G	194	ARG	2.9
1	B	157	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	148	TYR	2.9
1	C	193	VAL	2.8
1	B	147[A]	TYR	2.7
1	G	157	TYR	2.7
1	B	1	MET	2.6
1	E	206	LYS	2.6
1	G	202	PRO	2.6
1	C	148	TYR	2.5
1	E	44	GLU	2.5
1	C	157	TYR	2.5
1	E	207	MET	2.4
1	B	205	THR	2.4
1	G	204	PHE	2.4
1	G	198	ALA	2.3
1	G	214	THR	2.3
1	A	157	TYR	2.2
1	H	58	GLY	2.2
1	A	220	ASN	2.2
1	G	208	TYR	2.2
1	C	212	ALA	2.2
1	H	1	MET	2.1
1	B	85	GLY	2.1
1	F	103	GLU	2.1
1	F	78	ALA	2.1
1	F	209	ASP	2.1
1	D	207	MET	2.1
1	F	192	PRO	2.1
1	D	46	LEU	2.1
1	F	212	ALA	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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAP	H	501	48/48	0.21	0.74	40,46,71,73	0
2	NAP	D	500	48/48	0.19	0.71	33,44,69,72	0

## 6.5 Other polymers

There are no such residues in this entry.