



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:19 AM GMT

PDB ID : 2GM8  
Title : TenA Homolog/Thi-4 Thiaminase complexed with product 4-amino-5-hydroxymethyl-2-methylpyrimidine  
Authors : Sawaya, M.R.; Chan, S.; Han, G.W.; Perry, L.J.; Pashkov, I.  
Deposited on : 2006-04-06  
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.

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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

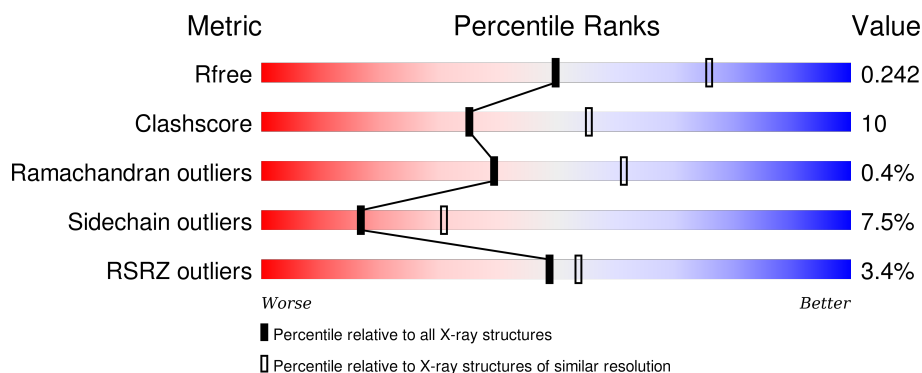
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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	221	<div> <div>2%</div> <div>78% 17% . .</div> </div>
1	B	221	<div> <div>%</div> <div>77% 16% . .</div> </div>
1	C	221	<div> <div>5%</div> <div>72% 22% . .</div> </div>
1	D	221	<div> <div>5%</div> <div>70% 24% . .</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	A	305	-	-	-	X
3	EDO	D	306	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7058 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 tenA homolog/Thi-4 Thiaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	1	0
			1738	1123	291	316	8			
1	B	213	Total	C	N	O	S	0	1	0
			1718	1111	287	312	8			
1	C	215	Total	C	N	O	S	0	0	0
			1730	1118	290	314	8			
1	D	217	Total	C	N	O	S	0	0	0
			1750	1130	296	316	8			

There are 40 discrepancies between the modelled and reference sequences:

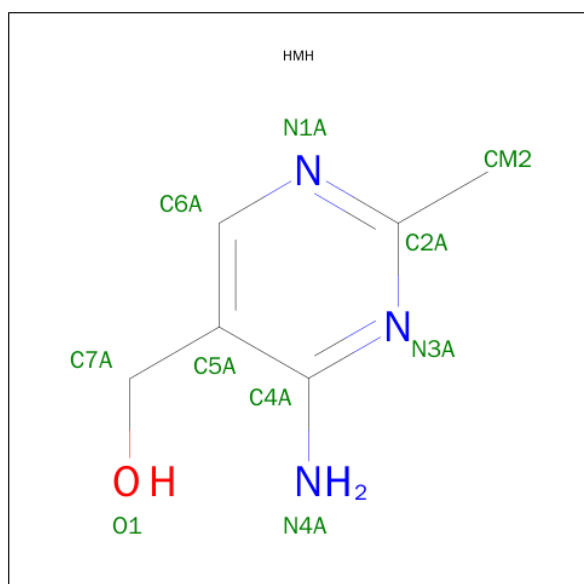
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	CLONING ARTIFACT	UNP Q8ZZM9
A	-7	ALA	-	CLONING ARTIFACT	UNP Q8ZZM9
A	-6	LEU	-	CLONING ARTIFACT	UNP Q8ZZM9
A	-5	HIS	-	CLONING ARTIFACT	UNP Q8ZZM9
A	-4	HIS	-	CLONING ARTIFACT	UNP Q8ZZM9
A	-3	HIS	-	CLONING ARTIFACT	UNP Q8ZZM9
A	-2	HIS	-	CLONING ARTIFACT	UNP Q8ZZM9
A	-1	HIS	-	CLONING ARTIFACT	UNP Q8ZZM9
A	0	HIS	-	CLONING ARTIFACT	UNP Q8ZZM9
A	1	GLY	-	CLONING ARTIFACT	UNP Q8ZZM9
B	-8	MET	-	CLONING ARTIFACT	UNP Q8ZZM9
B	-7	ALA	-	CLONING ARTIFACT	UNP Q8ZZM9
B	-6	LEU	-	CLONING ARTIFACT	UNP Q8ZZM9
B	-5	HIS	-	CLONING ARTIFACT	UNP Q8ZZM9
B	-4	HIS	-	CLONING ARTIFACT	UNP Q8ZZM9
B	-3	HIS	-	CLONING ARTIFACT	UNP Q8ZZM9
B	-2	HIS	-	CLONING ARTIFACT	UNP Q8ZZM9
B	-1	HIS	-	CLONING ARTIFACT	UNP Q8ZZM9
B	0	HIS	-	CLONING ARTIFACT	UNP Q8ZZM9
B	1	GLY	-	CLONING ARTIFACT	UNP Q8ZZM9
C	-8	MET	-	CLONING ARTIFACT	UNP Q8ZZM9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	ALA	-	CLONING ARTIFACT	UNP Q8ZZM9
C	-6	LEU	-	CLONING ARTIFACT	UNP Q8ZZM9
C	-5	HIS	-	CLONING ARTIFACT	UNP Q8ZZM9
C	-4	HIS	-	CLONING ARTIFACT	UNP Q8ZZM9
C	-3	HIS	-	CLONING ARTIFACT	UNP Q8ZZM9
C	-2	HIS	-	CLONING ARTIFACT	UNP Q8ZZM9
C	-1	HIS	-	CLONING ARTIFACT	UNP Q8ZZM9
C	0	HIS	-	CLONING ARTIFACT	UNP Q8ZZM9
C	1	GLY	-	CLONING ARTIFACT	UNP Q8ZZM9
D	-8	MET	-	CLONING ARTIFACT	UNP Q8ZZM9
D	-7	ALA	-	CLONING ARTIFACT	UNP Q8ZZM9
D	-6	LEU	-	CLONING ARTIFACT	UNP Q8ZZM9
D	-5	HIS	-	CLONING ARTIFACT	UNP Q8ZZM9
D	-4	HIS	-	CLONING ARTIFACT	UNP Q8ZZM9
D	-3	HIS	-	CLONING ARTIFACT	UNP Q8ZZM9
D	-2	HIS	-	CLONING ARTIFACT	UNP Q8ZZM9
D	-1	HIS	-	CLONING ARTIFACT	UNP Q8ZZM9
D	0	HIS	-	CLONING ARTIFACT	UNP Q8ZZM9
D	1	GLY	-	CLONING ARTIFACT	UNP Q8ZZM9

- Molecule 2 is 4-AMINO-5-HYDROXYMETHYL-2-METHYLPYRIMIDINE (three-letter code: HMH) (formula: C<sub>6</sub>H<sub>9</sub>N<sub>3</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	3	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			10	6	3	1		
2	C	1	Total	C	N	O	0	0
			10	6	3	1		
2	D	1	Total	C	N	O	0	0
			10	6	3	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



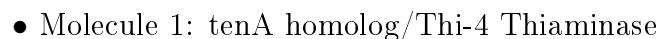
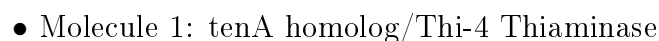
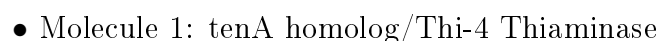
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

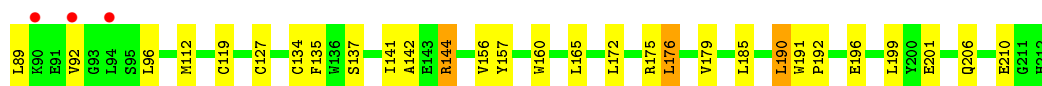
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total	O	0	0
			18	18		
4	B	25	Total	O	0	0
			25	25		
4	C	16	Total	O	0	0
			16	16		
4	D	15	Total	O	0	0
			15	15		



- Molecule 1: tenA homolog/Thi-4 Thiaminase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.65Å 94.29Å 73.20Å 90.00° 113.65° 90.00°	Depositor
Resolution (Å)	67.12 – 2.50 67.05 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (67.12-2.50) 99.1 (67.05-2.50)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.53 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.187 , 0.237 0.194 , 0.242	Depositor DCC
$R_{free}$ test set	1533 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.8	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.8	EDS
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 30264 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7058	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.66% 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

### 5.1 Standard geometry

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

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	0.34	0/1787	0.67	0/2423
1	B	0.34	0/1767	0.68	1/2395 (0.0%)
1	C	0.31	0/1778	0.63	1/2411 (0.0%)
1	D	0.32	0/1800	0.65	0/2441
All	All	0.33	0/7132	0.66	2/9670 (0.0%)

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	1	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	212	HIS	N-CA-C	5.74	126.49	111.00
1	C	165	LEU	CA-CB-CG	5.14	127.12	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	212	HIS	CA

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	1738	0	1695	30	0
1	B	1718	0	1687	25	0
1	C	1730	0	1688	37	0
1	D	1750	0	1702	48	0
2	A	10	0	9	2	0
2	B	10	0	9	2	0
2	C	10	0	9	2	0
2	D	10	0	9	2	0
3	A	4	0	6	0	0
3	D	4	0	6	0	0
4	A	18	0	0	0	0
4	B	25	0	0	2	0
4	C	16	0	0	0	0
4	D	15	0	0	2	0
All	All	7058	0	6820	135	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 10.

All (135) 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:D:58:ALA:HB1	1:D:71:LEU:CD1	2.01	0.91
1:D:58:ALA:HB1	1:D:71:LEU:HD13	1.59	0.82
1:B:73:LEU:HD12	1:B:172:LEU:HG	1.62	0.80
1:D:37:LYS:O	1:D:41:LEU:HD22	1.79	0.80
1:C:37:LYS:O	1:C:41:LEU:HD22	1.83	0.77
1:C:49:ASN:ND2	1:C:112:MET:SD	2.56	0.77
1:D:206:GLN:NE2	1:D:210:GLU:OE2	2.19	0.74
1:A:16:ARG:HH11	1:A:16:ARG:HG2	1.54	0.71
1:C:132:LEU:HD22	1:C:180:LEU:HD12	1.72	0.71
1:D:58:ALA:CB	1:D:71:LEU:CD1	2.69	0.70
1:C:82:MET:O	1:C:86:GLU:HG3	1.93	0.69
1:D:26:LEU:HD13	1:D:160:TRP:CZ3	2.28	0.69
1:B:54:LEU:CD2	1:B:131:LEU:HD13	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:THR:O	1:C:73:LEU:HD23	1.94	0.68
1:D:72:GLU:O	1:D:76:GLY:N	2.21	0.66
1:D:175:ARG:O	1:D:179:VAL:HG23	1.97	0.64
1:C:37:LYS:HE2	1:C:92:VAL:HG12	1.78	0.63
1:C:142:ALA:HB1	1:C:165:LEU:HD22	1.81	0.62
1:C:192:PRO:O	1:C:196:GLU:HG2	2.01	0.61
1:C:78:VAL:HG13	1:D:68:LYS:HE2	1.83	0.61
1:B:54:LEU:HD21	1:B:131:LEU:HD13	1.81	0.60
1:A:37:LYS:O	1:A:41:LEU:HD22	2.01	0.60
1:D:-3:HIS:CD2	1:D:-3:HIS:H	2.19	0.60
1:A:192:PRO:O	1:A:196:GLU:HG2	2.03	0.59
1:A:119:CYS:HA	1:A:127:CYS:SG	2.43	0.59
1:C:92:VAL:HG12	1:C:92:VAL:O	2.02	0.59
1:C:28:ALA:HB3	1:C:30:THR:HG22	1.86	0.58
1:B:30:THR:CG2	1:B:30:THR:O	2.50	0.58
1:C:88:LEU:O	1:C:92:VAL:HG23	2.03	0.58
1:D:192:PRO:O	1:D:196:GLU:HG2	2.03	0.58
1:D:-4:HIS:O	1:D:-1:HIS:HB2	2.03	0.57
1:B:119:CYS:HA	1:B:127:CYS:SG	2.45	0.57
1:D:61:ALA:HB3	1:D:67:MET:HB2	1.86	0.56
1:C:58:ALA:HB1	1:C:71:LEU:HD13	1.86	0.56
1:D:92:VAL:O	1:D:92:VAL:CG1	2.52	0.56
1:C:183:SER:HB2	1:C:185:LEU:HD13	1.87	0.55
1:D:26:LEU:HD23	1:D:26:LEU:O	2.06	0.55
1:A:73:LEU:HD12	1:A:172:LEU:HG	1.88	0.55
1:B:192:PRO:O	1:B:196:GLU:HG2	2.07	0.55
1:B:3:THR:HG23	1:B:181:ASP:OD1	2.07	0.54
1:A:30:THR:O	1:A:30:THR:CG2	2.54	0.54
1:B:106:ARG:HD3	1:D:199:LEU:HD13	1.89	0.53
1:B:54:LEU:HD23	1:B:131:LEU:HD13	1.90	0.53
1:B:36:PHE:CE2	1:B:40:LEU:HD11	2.43	0.53
1:B:92:VAL:O	1:B:92:VAL:CG1	2.57	0.53
1:D:137:SER:O	1:D:141:ILE:HG13	2.09	0.53
1:C:77:THR:O	1:C:77:THR:CG2	2.56	0.53
1:B:5:GLU:OE1	1:B:8:ARG:NH1	2.40	0.53
1:D:66:LEU:HD22	4:D:321:HOH:O	2.08	0.53
1:D:58:ALA:CB	1:D:71:LEU:HD12	2.38	0.52
1:A:54:LEU:CD2	1:A:131:LEU:HD13	2.39	0.52
1:C:61:ALA:HB3	1:C:67:MET:HB2	1.91	0.51
1:A:18:LEU:HD13	1:A:144:ARG:NH1	2.26	0.51
1:B:30:THR:HG22	1:B:30:THR:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:VAL:HG11	1:C:141:ILE:HG23	1.93	0.51
1:A:211:GLY:O	1:A:212:HIS:OXT	2.29	0.51
1:D:80:GLY:O	1:D:81:GLU:C	2.49	0.51
1:D:49:ASN:ND2	1:D:112:MET:SD	2.83	0.51
1:D:40:LEU:HB3	1:D:89:LEU:HD21	1.94	0.50
1:D:92:VAL:HG12	1:D:92:VAL:O	2.12	0.50
1:C:25:GLU:HA	1:C:30:THR:HG23	1.92	0.50
1:C:170:ARG:O	1:C:174:GLU:HG2	2.12	0.50
1:A:207:ALA:HA	1:A:212:HIS:CD2	2.46	0.50
1:A:201:GLU:OE2	2:A:301:HMH:N1A	2.45	0.50
1:D:80:GLY:O	1:D:83:ALA:N	2.45	0.49
1:B:43:ASP:OD1	2:B:302:HMH:N3A	2.45	0.49
1:D:-3:HIS:H	1:D:-3:HIS:HD2	1.59	0.49
1:C:73:LEU:CD1	1:C:172:LEU:HG	2.43	0.49
1:B:142:ALA:HB1	1:B:165:LEU:HD13	1.95	0.49
1:D:134:CYS:O	2:D:304:HMH:HC6	2.13	0.49
1:A:68:LYS:NZ	1:B:86:GLU:OE2	2.35	0.49
1:A:26:LEU:HD13	1:A:160:TRP:CZ3	2.47	0.48
1:A:106:ARG:HD3	1:C:199:LEU:HD13	1.94	0.48
1:D:185:LEU:HD23	1:D:190:LEU:HD11	1.95	0.48
1:B:166:SER:O	1:B:170:ARG:HG3	2.13	0.48
1:C:23:VAL:CG1	1:C:141:ILE:HG23	2.44	0.48
1:C:88:LEU:HD21	1:C:160:TRP:HA	1.95	0.48
1:C:26:LEU:HD13	1:C:160:TRP:CZ3	2.48	0.48
1:A:16:ARG:NH1	1:A:16:ARG:HG2	2.22	0.48
1:D:86:GLU:HG2	1:D:96:LEU:HD21	1.95	0.48
1:C:134:CYS:O	2:C:303:HMH:HC6	2.14	0.47
1:D:26:LEU:CD2	1:D:26:LEU:C	2.83	0.47
1:C:191:TRP:HB3	1:C:192:PRO:HD3	1.96	0.47
1:D:201:GLU:OE2	2:D:304:HMH:N1A	2.49	0.46
1:D:73:LEU:N	1:D:73:LEU:CD1	2.78	0.46
1:A:43:ASP:OD1	2:A:301:HMH:N3A	2.49	0.45
1:D:23:VAL:HG11	1:D:141:ILE:HG23	1.99	0.45
1:C:81:GLU:OE2	2:C:303:HMH:HC71	2.17	0.45
1:A:54:LEU:HD21	1:A:131:LEU:HD13	1.97	0.45
1:B:92:VAL:O	1:B:92:VAL:HG13	2.17	0.44
1:A:133:PRO:HG2	1:A:197:ALA:HB3	1.98	0.44
1:A:92:VAL:O	1:A:92:VAL:CG1	2.65	0.44
1:D:23:VAL:CG1	1:D:141:ILE:HG23	2.47	0.44
1:D:144:ARG:HD3	4:D:308:HOH:O	2.16	0.44
1:D:26:LEU:CD2	1:D:26:LEU:O	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:HIS:NE2	1:D:206:GLN:OE1	2.43	0.44
1:A:71:LEU:HA	1:A:71:LEU:HD12	1.74	0.44
1:C:3:THR:HG23	1:C:181:ASP:OD1	2.18	0.44
1:D:156:VAL:HG23	1:D:157:TYR:CD1	2.53	0.43
1:C:169:TYR:O	1:C:173:VAL:HG23	2.18	0.43
1:C:18:LEU:HD13	1:C:144:ARG:NH1	2.33	0.43
1:A:30:THR:O	1:A:30:THR:HG23	2.18	0.43
1:D:142:ALA:HB1	1:D:165:LEU:HD22	2.01	0.43
1:D:69:THR:O	1:D:72:GLU:N	2.48	0.43
1:C:20:HIS:HA	1:C:21:PRO:HD3	1.94	0.43
1:B:42:GLN:HG2	4:B:326:HOH:O	2.19	0.43
1:C:22:PHE:O	1:C:26:LEU:HB2	2.19	0.42
1:D:73:LEU:HD21	1:D:176:LEU:HD11	2.00	0.42
1:D:191:TRP:HB3	1:D:192:PRO:HD3	2.01	0.42
1:A:-1:HIS:HA	1:A:4:GLY:HA3	2.02	0.42
1:C:73:LEU:CD2	1:C:73:LEU:H	2.32	0.42
1:A:20:HIS:CG	1:A:21:PRO:HD2	2.54	0.42
1:B:28:ALA:HB2	4:B:320:HOH:O	2.19	0.42
1:A:61:ALA:HB3	1:A:67:MET:HB2	2.01	0.42
1:D:26:LEU:CD2	1:D:157:TYR:HB3	2.48	0.42
1:A:21:PRO:O	1:A:25:GLU:HG3	2.20	0.42
1:D:135:PHE:CE2	1:D:172:LEU:HD23	2.55	0.42
1:D:119:CYS:HA	1:D:127:CYS:SG	2.59	0.42
1:D:206:GLN:HG3	1:D:210:GLU:OE2	2.19	0.42
1:B:191:TRP:HB3	1:B:192:PRO:HD3	2.02	0.42
1:A:88:LEU:CD1	1:A:159:LYS:HD3	2.50	0.42
1:B:129:ALA:HB2	1:B:190:LEU:HG	2.00	0.42
1:B:81:GLU:OE2	2:B:302:HMH:N4A	2.46	0.42
1:C:151:GLU:O	1:C:151:GLU:HG3	2.20	0.41
1:B:62:PRO:HG2	1:B:66:LEU:HD23	2.02	0.41
1:A:132:LEU:N	1:A:133:PRO:CD	2.84	0.41
1:A:64:VAL:HG12	1:A:68:LYS:HE2	2.03	0.41
1:A:66:LEU:HG	1:A:124:PHE:CE2	2.54	0.41
1:D:37:LYS:HE3	1:D:92:VAL:HG13	2.03	0.40
1:D:22:PHE:CZ	1:D:31:LEU:HD21	2.55	0.40
1:C:55:SER:OG	1:D:71:LEU:HD11	2.21	0.40
1:A:54:LEU:HD23	1:A:131:LEU:HD13	2.03	0.40
1:B:74:ALA:O	1:B:77:THR:HB	2.21	0.40
1:C:92:VAL:O	1:C:92:VAL:CG1	2.70	0.40
1:C:77:THR:O	1:C:77:THR:HG22	2.21	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	216/221 (98%)	214 (99%)	2 (1%)	0	100	100
1	B	212/221 (96%)	210 (99%)	2 (1%)	0	100	100
1	C	213/221 (96%)	208 (98%)	4 (2%)	1 (0%)	34	55
1	D	215/221 (97%)	210 (98%)	3 (1%)	2 (1%)	21	37
All	All	856/884 (97%)	842 (98%)	11 (1%)	3 (0%)	39	61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	0	HIS
1	C	-1	HIS
1	D	81	GLU

### 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	173/179 (97%)	160 (92%)	13 (8%)	17	31
1	B	173/179 (97%)	157 (91%)	16 (9%)	11	21
1	C	174/179 (97%)	164 (94%)	10 (6%)	25	46
1	D	176/179 (98%)	162 (92%)	14 (8%)	15	28
All	All	696/716 (97%)	643 (92%)	53 (8%)	17	30

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	26	LEU
1	A	30	THR
1	A	41	LEU
1	A	66	LEU
1	A	71	LEU
1	A	73	LEU
1	A	88	LEU
1	A	144	ARG
1	A	174	GLU
1	A	185	LEU
1	A	190	LEU
1	A	210	GLU
1	B	5	GLU
1	B	26	LEU
1	B	41	LEU
1	B	60[A]	ARG
1	B	60[B]	ARG
1	B	65	ASP
1	B	66	LEU
1	B	71	LEU
1	B	73	LEU
1	B	88	LEU
1	B	92	VAL
1	B	144	ARG
1	B	165	LEU
1	B	185	LEU
1	B	190	LEU
1	B	212	HIS
1	C	5	GLU
1	C	26	LEU
1	C	30	THR
1	C	41	LEU
1	C	66	LEU
1	C	134	CYS
1	C	144	ARG
1	C	176	LEU
1	C	190	LEU
1	C	212	HIS
1	D	-3	HIS
1	D	5	GLU
1	D	8	ARG
1	D	16	ARG

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Mol	Chain	Res	Type
1	D	26	LEU
1	D	41	LEU
1	D	45	ASN
1	D	60	ARG
1	D	66	LEU
1	D	73	LEU
1	D	79	THR
1	D	144	ARG
1	D	176	LEU
1	D	190	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-1	HIS
1	A	212	HIS
1	C	-2	HIS
1	C	212	HIS
1	D	-3	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

6 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	HMH	A	301	-	10,10,10	0.79	0	12,13,13	1.91	5 (41%)
3	EDO	A	305	-	3,3,3	0.52	0	2,2,2	0.27	0
2	HMH	B	302	-	10,10,10	0.77	0	12,13,13	1.79	5 (41%)
2	HMH	C	303	-	10,10,10	0.82	0	12,13,13	1.98	7 (58%)
2	HMH	D	304	-	10,10,10	0.80	0	12,13,13	1.96	5 (41%)
3	EDO	D	306	-	3,3,3	0.56	0	2,2,2	0.13	0

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	HMH	A	301	-	-	0/2/2/2	0/1/1/1
3	EDO	A	305	-	-	0/1/1/1	0/0/0/0
2	HMH	B	302	-	-	0/2/2/2	0/1/1/1
2	HMH	C	303	-	-	0/2/2/2	0/1/1/1
2	HMH	D	304	-	-	0/2/2/2	0/1/1/1
3	EDO	D	306	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	HMH	N1A-C2A-N3A	-2.81	120.40	125.60
2	D	304	HMH	N1A-C2A-N3A	-2.79	120.44	125.60
2	C	303	HMH	N1A-C2A-N3A	-2.64	120.72	125.60
2	B	302	HMH	N1A-C2A-N3A	-2.45	121.06	125.60
2	D	304	HMH	C5A-C6A-N1A	-2.23	120.00	123.86
2	C	303	HMH	C5A-C6A-N1A	-2.13	120.15	123.86
2	A	301	HMH	C5A-C4A-N4A	-2.07	119.21	122.25
2	C	303	HMH	C7A-C5A-C6A	-2.05	115.44	119.31
2	B	302	HMH	C5A-C6A-N1A	-2.00	120.38	123.86
2	D	304	HMH	CM2-C2A-N3A	2.01	120.62	117.20
2	B	302	HMH	N4A-C4A-N3A	2.03	119.90	116.95
2	C	303	HMH	C6A-C5A-C4A	2.09	118.71	115.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	302	HMH	CM2-C2A-N1A	2.10	119.55	117.03
2	C	303	HMH	N4A-C4A-N3A	2.20	120.14	116.95
2	A	301	HMH	CM2-C2A-N3A	2.24	121.01	117.20
2	D	304	HMH	N4A-C4A-N3A	2.48	120.55	116.95
2	B	302	HMH	C6A-N1A-C2A	2.53	120.19	115.77
2	A	301	HMH	C6A-N1A-C2A	2.75	120.58	115.77
2	C	303	HMH	CM2-C2A-N3A	2.84	122.04	117.20
2	C	303	HMH	C6A-N1A-C2A	2.90	120.85	115.77
2	A	301	HMH	N4A-C4A-N3A	3.03	121.34	116.95
2	D	304	HMH	C6A-N1A-C2A	3.17	121.31	115.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	HMH	2	0
2	B	302	HMH	2	0
2	C	303	HMH	2	0
2	D	304	HMH	2	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	217/221 (98%)	0.07	5 (2%) 64 67	17, 30, 57, 144	0
1	B	213/221 (96%)	0.04	2 (0%) 85 88	17, 29, 50, 91	0
1	C	215/221 (97%)	0.19	10 (4%) 35 40	16, 32, 56, 125	0
1	D	217/221 (98%)	0.26	12 (5%) 29 32	17, 32, 57, 155	0
All	All	862/884 (97%)	0.14	29 (3%) 49 54	16, 31, 56, 155	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	-4	HIS	12.5
1	A	-3	HIS	9.5
1	D	-3	HIS	7.8
1	D	-2	HIS	6.9
1	C	94	LEU	5.1
1	C	0	HIS	4.9
1	C	-2	HIS	4.4
1	A	-2	HIS	4.0
1	A	-1	HIS	3.7
1	B	212	HIS	3.6
1	D	71	LEU	3.4
1	C	97	ARG	3.3
1	B	0	HIS	3.1
1	C	212	HIS	2.9
1	D	75	TYR	2.8
1	C	-1	HIS	2.7
1	C	150	ARG	2.7
1	C	92	VAL	2.6
1	D	0	HIS	2.6
1	A	23	VAL	2.5
1	C	181	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	92	VAL	2.4
1	D	-1	HIS	2.4
1	D	79	THR	2.4
1	D	94	LEU	2.3
1	A	212	HIS	2.3
1	C	71	LEU	2.1
1	D	77	THR	2.0
1	D	90	LYS	2.0

## 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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	A	305	4/4	0.87	0.20	5.10	45,46,50,55	0
3	EDO	D	306	4/4	0.76	0.23	4.28	40,51,58,59	0
2	HMH	D	304	10/10	0.94	0.17	0.68	22,37,45,49	0
2	HMH	C	303	10/10	0.94	0.14	-0.68	29,36,49,63	0
2	HMH	A	301	10/10	0.97	0.12	-0.92	11,17,26,33	0
2	HMH	B	302	10/10	0.98	0.10	-4.77	13,18,23,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.