



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 24, 2017 – 11:26 PM EST

PDB ID : 1N97
Title : Crystal Structure of CYP175A1 from *Thermus thermophilus* strain HB27
Authors : Yano, J.K.; Blasco, F.; Li, H.; Schmid, R.D.; Henne, A.; Poulos, T.L.
Deposited on : 2002-11-22
Resolution : 1.80 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
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) : rb-20028442

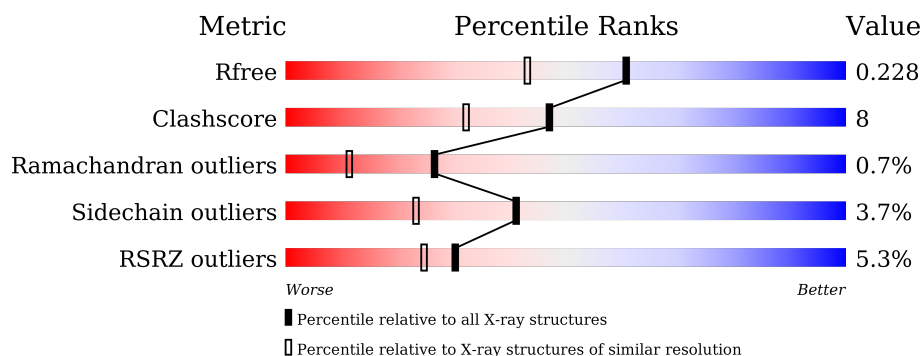
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 ≥ 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	389	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>18%</div> <div>..</div> </div> </div>
1	B	389	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>..</div> </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
2	SRT	A	601	X	-	-	X
2	SRT	B	602	X	-	-	X
4	EDO	A	715	-	-	-	X
4	EDO	A	717	-	-	-	X
4	EDO	B	704	-	-	-	X
4	EDO	B	707	-	-	-	X
4	EDO	B	708	-	-	-	X
4	EDO	B	709	-	-	-	X

2 Entry composition [i](#)

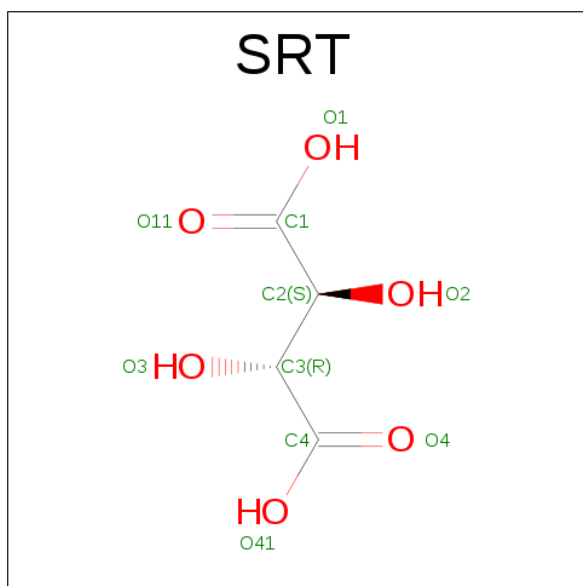
There are 5 unique types of molecules in this entry. The entry contains 6832 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CYP175A1.

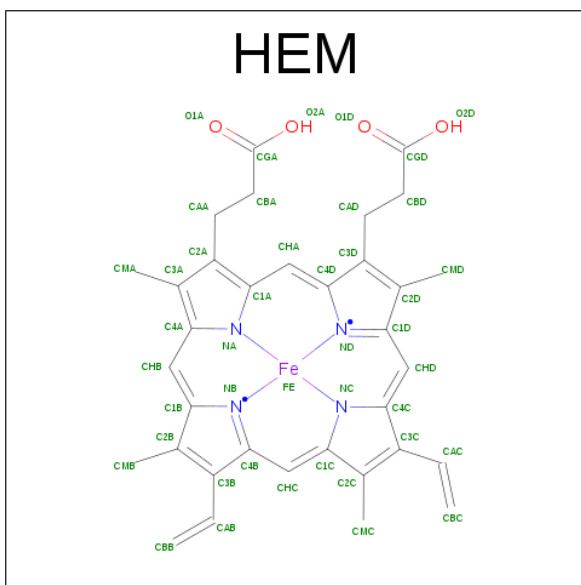
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	0	0
			3052	1972	557	518	5			
1	B	385	Total	C	N	O	S	27	0	0
			3074	1985	560	524	5			

- Molecule 2 is S,R MESO-TARTARIC ACID (three-letter code: SRT) (formula: C₄H₆O₆).



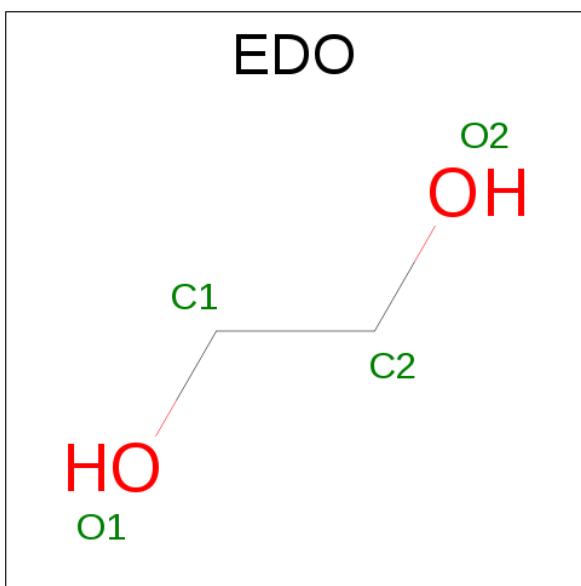
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	4	6		
2	B	1	Total	C	O	0	0
			10	4	6		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



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

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

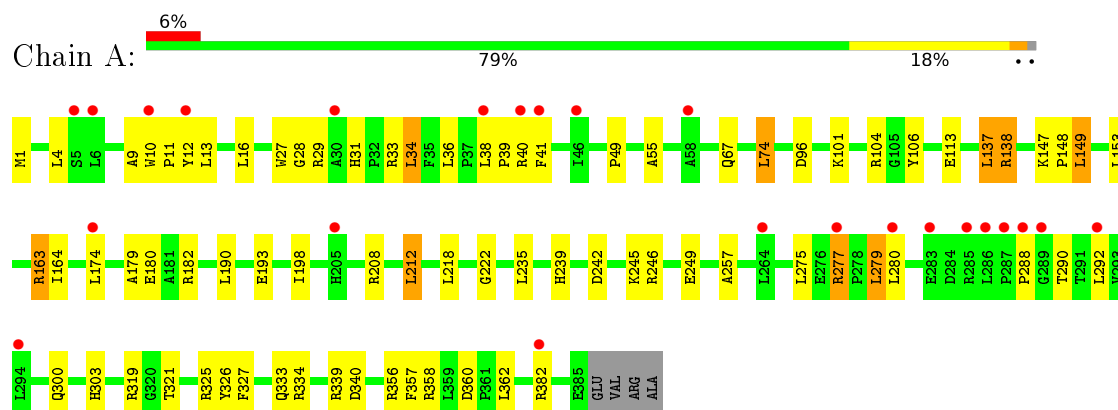
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	206	Total O 206 206	0	0
5	B	322	Total O 322 322	0	0

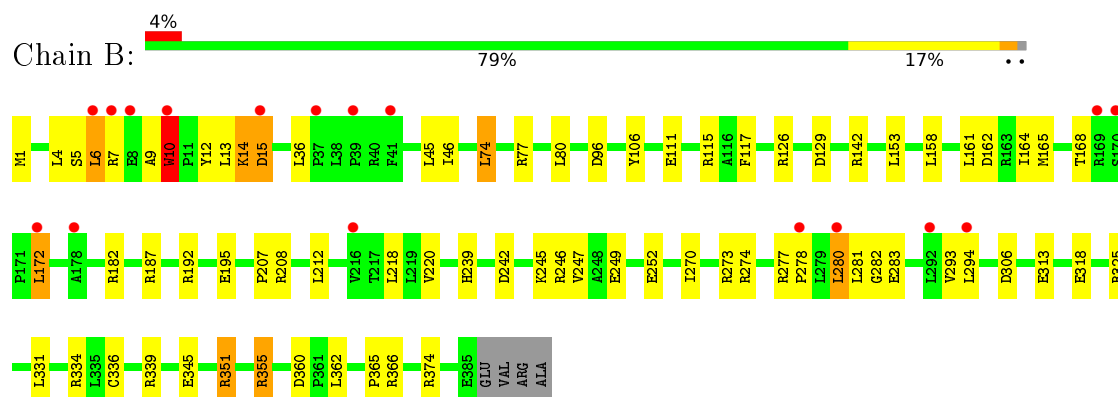
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: CYP175A1



• Molecule 1: CYP175A1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.54Å 90.70Å 74.52Å 90.00° 99.68° 90.00°	Depositor
Resolution (Å)	19.99 – 1.80 19.99 – 1.80	Depositor EDS
% Data completeness (in resolution range)	92.0 (19.99-1.80) 92.0 (19.99-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.92 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.182 , 0.222 0.190 , 0.228	Depositor DCC
R_{free} test set	3639 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6832	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: HEM, EDO, SRT

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	1.13	5/3136 (0.2%)	1.02	8/4263 (0.2%)
1	B	1.38	8/3158 (0.3%)	1.19	28/4288 (0.7%)
All	All	1.26	13/6294 (0.2%)	1.11	36/8551 (0.4%)

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	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	10	TRP	C-N	-12.85	1.09	1.34
1	B	13	LEU	C-N	10.64	1.58	1.34
1	B	313	GLU	CD-OE2	-10.45	1.14	1.25
1	B	313	GLU	CD-OE1	10.29	1.36	1.25
1	B	106	TYR	CE2-CZ	-7.53	1.28	1.38
1	B	345	GLU	CD-OE2	-6.77	1.18	1.25
1	A	319	ARG	CG-CD	6.61	1.68	1.51
1	B	325	ARG	CB-CG	-6.07	1.36	1.52
1	A	257	ALA	CA-CB	5.79	1.64	1.52
1	A	106	TYR	CG-CD2	5.75	1.46	1.39
1	A	326	TYR	CD2-CE2	5.53	1.47	1.39
1	B	111	GLU	CD-OE1	-5.44	1.19	1.25
1	A	321	THR	CB-CG2	-5.12	1.35	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	334	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	B	334	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	B	187	ARG	NE-CZ-NH1	8.97	124.78	120.30
1	B	162	ASP	CB-CG-OD2	8.88	126.29	118.30
1	B	355	ARG	NE-CZ-NH1	8.65	124.62	120.30
1	B	192	ARG	NE-CZ-NH1	8.49	124.54	120.30
1	A	242	ASP	CB-CG-OD2	8.39	125.85	118.30
1	A	246	ARG	NE-CZ-NH1	7.61	124.10	120.30
1	A	360	ASP	CB-CG-OD2	7.33	124.89	118.30
1	B	306	ASP	CB-CG-OD2	6.98	124.58	118.30
1	B	273	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	B	96	ASP	CB-CG-OD2	6.67	124.30	118.30
1	B	15	ASP	CB-CG-OD2	6.55	124.19	118.30
1	B	10	TRP	O-C-N	-6.48	108.79	121.10
1	A	104	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	B	129	ASP	CB-CG-OD2	6.21	123.89	118.30
1	B	182	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	B	351	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	B	187	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	B	360	ASP	CB-CG-OD2	5.96	123.67	118.30
1	B	366	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	374	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	B	115	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	246	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	B	331	LEU	CB-CG-CD2	-5.41	101.80	111.00
1	B	355	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	A	334	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	B	1	MET	CG-SD-CE	5.27	108.63	100.20
1	B	212	LEU	CB-CG-CD1	-5.19	102.17	111.00
1	A	96	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	246	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	80	LEU	CB-CG-CD1	-5.16	102.23	111.00
1	B	339	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	242	ASP	CB-CG-OD2	5.05	122.85	118.30
1	B	77	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	340	ASP	CB-CG-OD2	5.04	122.84	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	10	TRP	Mainchain

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	3052	0	3082	60	0
1	B	3074	0	3119	34	1
2	A	10	0	5	1	0
2	B	10	0	4	0	0
3	A	43	0	30	1	0
3	B	43	0	30	1	0
4	A	28	0	42	3	0
4	B	44	0	66	9	0
5	A	206	0	0	3	1
5	B	322	0	0	6	1
All	All	6832	0	6378	95	2

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 8.

All (95) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:LEU:HD21	5:A:734:HOH:O	1.73	0.87
1:A:245:LYS:NZ	1:A:249:GLU:OE2	2.13	0.81
1:A:280:LEU:HD23	1:A:280:LEU:H	1.52	0.74
1:A:74:LEU:HB2	1:A:164:ILE:CD1	2.17	0.74
1:B:74:LEU:HD12	1:B:161:LEU:HG	1.70	0.73
1:A:292:LEU:N	1:A:292:LEU:HD12	2.05	0.72
1:A:300:GLN:HE21	1:A:327:PHE:H	1.37	0.72
1:A:138:ARG:HB3	1:A:138:ARG:HH11	1.55	0.71
1:B:195:GLU:OE2	1:B:208:ARG:NH2	2.24	0.70
1:A:249:GLU:OE1	5:A:764:HOH:O	2.11	0.67
1:A:163:ARG:HD3	1:A:180:GLU:OE2	1.95	0.66
1:A:280:LEU:CD2	1:A:280:LEU:H	2.08	0.66
4:B:709:EDO:H21	5:B:980:HOH:O	1.97	0.64
1:A:113:GLU:OE2	1:A:138:ARG:NH1	2.30	0.64
1:B:280:LEU:HD23	1:B:280:LEU:H	1.63	0.62
1:A:10:TRP:HZ2	1:A:39:PRO:HG2	1.63	0.62
1:B:351:ARG:NH2	1:B:355:ARG:HH21	1.96	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:GLU:OE2	1:A:138:ARG:CZ	2.48	0.61
1:A:74:LEU:HB2	1:A:164:ILE:HD12	1.81	0.60
1:A:275:LEU:HD13	1:A:292:LEU:HD11	1.84	0.60
1:A:198:ILE:HD13	1:A:212:LEU:HD13	1.84	0.59
1:A:292:LEU:N	1:A:292:LEU:CD1	2.66	0.58
1:A:138:ARG:CB	1:A:138:ARG:HH11	2.15	0.58
1:A:358:ARG:HG2	1:A:358:ARG:HH11	1.68	0.58
1:B:9:ALA:O	1:B:14:LYS:HB2	2.05	0.57
1:A:382:ARG:NE	5:A:898:HOH:O	2.37	0.57
1:A:10:TRP:CZ2	1:A:39:PRO:HG2	2.39	0.57
1:A:67:GLN:HE21	4:A:715:EDO:H21	1.69	0.57
1:A:49:PRO:HD3	1:A:303:HIS:CD2	2.39	0.57
1:A:239:HIS:HE1	1:A:362:LEU:O	1.88	0.57
1:A:163:ARG:HE	1:A:163:ARG:HA	1.69	0.56
1:A:275:LEU:HD13	1:A:292:LEU:CD1	2.35	0.56
1:A:358:ARG:NH1	1:A:358:ARG:HG2	2.20	0.56
1:A:300:GLN:NE2	1:A:327:PHE:H	2.01	0.56
1:A:40:ARG:O	1:A:41:PHE:CD1	2.58	0.56
1:A:10:TRP:HB2	1:A:11:PRO:HD3	1.87	0.56
1:A:13:LEU:HD13	1:A:13:LEU:C	2.26	0.55
1:A:356:ARG:NH1	1:A:357:PHE:CZ	2.75	0.55
1:B:351:ARG:HG3	5:B:879:HOH:O	2.07	0.55
1:B:46:ILE:HD13	1:B:281:LEU:HD21	1.89	0.54
1:A:275:LEU:HD11	1:A:279:LEU:HD12	1.89	0.54
1:B:355:ARG:NH1	5:B:903:HOH:O	2.39	0.54
1:A:153:LEU:HD12	1:A:190:LEU:HD12	1.89	0.54
1:B:10:TRP:CD1	1:B:10:TRP:N	2.78	0.51
1:B:239:HIS:HE1	1:B:362:LEU:O	1.94	0.51
1:B:164:ILE:O	1:B:168:THR:HG23	2.10	0.51
1:A:275:LEU:HD22	1:A:290:THR:HB	1.93	0.51
1:A:1:MET:HE2	1:A:34:LEU:C	2.31	0.50
1:B:172:LEU:N	1:B:172:LEU:HD12	2.28	0.49
1:B:142:ARG:HG2	5:B:982:HOH:O	2.12	0.48
1:B:351:ARG:HH21	1:B:355:ARG:HH21	1.60	0.48
1:A:138:ARG:HH11	1:A:138:ARG:CG	2.25	0.48
1:B:207:PRO:HA	4:B:703:EDO:H11	1.94	0.48
1:B:245:LYS:HZ3	1:B:249:GLU:CD	2.17	0.48
1:A:222:GLY:HA3	3:A:602:HEM:HBC2	1.96	0.48
1:B:45:LEU:HD23	1:B:293:VAL:HB	1.97	0.47
1:B:5:SER:C	1:B:7:ARG:H	2.18	0.47
1:A:29:ARG:HG2	1:A:29:ARG:HH11	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HB2	1:A:33:ARG:CB	2.45	0.47
1:B:270:ILE:HD13	1:B:294:LEU:O	2.15	0.46
1:B:4:LEU:HD12	1:B:36:LEU:HG	1.97	0.46
1:B:220:VAL:HA	4:B:710:EDO:H12	1.97	0.46
1:B:158:LEU:CD2	4:B:710:EDO:H22	2.46	0.46
1:B:158:LEU:HG	4:B:710:EDO:H22	1.98	0.46
1:A:163:ARG:NH1	1:A:180:GLU:OE2	2.35	0.46
1:B:117:PHE:CD1	4:B:707:EDO:H21	2.51	0.46
1:B:252:GLU:CD	5:B:970:HOH:O	2.55	0.45
1:B:277:ARG:HB2	1:B:278:PRO:CD	2.46	0.45
1:A:239:HIS:CE1	1:A:362:LEU:O	2.70	0.45
1:A:138:ARG:HA	1:A:148:PRO:HB3	1.98	0.44
1:A:28:GLY:HA2	1:A:31:HIS:O	2.17	0.44
1:A:137:LEU:HD22	1:A:149:LEU:HB2	1.98	0.44
1:A:333:GLN:HE22	4:A:714:EDO:H21	1.82	0.44
1:A:36:LEU:HB3	1:A:38:LEU:CD2	2.47	0.44
1:A:29:ARG:HG2	1:A:29:ARG:NH1	2.32	0.43
1:A:356:ARG:HG2	1:A:356:ARG:HH11	1.83	0.43
1:A:174:LEU:HG	1:A:174:LEU:O	2.19	0.43
1:B:126:ARG:HH22	4:B:708:EDO:H21	1.84	0.43
1:B:117:PHE:CG	4:B:707:EDO:H21	2.54	0.43
1:B:247:VAL:O	1:B:351:ARG:HD2	2.18	0.43
1:A:55:ALA:HB1	1:A:292:LEU:HD23	2.01	0.43
1:A:179:ALA:HA	1:A:182:ARG:HH11	1.85	0.42
1:A:4:LEU:HD13	1:A:12:TYR:HD1	1.83	0.42
1:A:101:LYS:HG3	4:A:717:EDO:H11	2.01	0.42
1:B:245:LYS:NZ	1:B:249:GLU:OE1	2.53	0.42
1:B:142:ARG:HD3	5:B:934:HOH:O	2.20	0.42
1:A:16:LEU:HD21	1:A:27:TRP:CZ3	2.55	0.41
1:A:153:LEU:HA	1:A:193:GLU:OE2	2.19	0.41
1:B:336:CYS:HA	3:B:603:HEM:CHA	2.50	0.41
1:B:117:PHE:CE1	4:B:707:EDO:H12	2.56	0.41
1:A:9:ALA:HB1	1:A:38:LEU:HD22	2.02	0.41
1:A:339:ARG:HH22	2:A:601:SRT:C4	2.34	0.41
1:A:138:ARG:NH1	1:A:138:ARG:CG	2.83	0.41
1:A:277:ARG:HA	1:A:288:PRO:HB3	2.02	0.41
1:B:274:ARG:HG2	1:B:274:ARG:HH11	1.87	0.40

All (2) 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)
5:B:748:HOH:O	5:B:1016:HOH:O[2_645]	1.70	0.50
1:B:252:GLU:OE1	5:A:867:HOH:O[2_656]	2.10	0.10

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	383/389 (98%)	375 (98%)	7 (2%)	1 (0%)	46	29
1	B	383/389 (98%)	368 (96%)	11 (3%)	4 (1%)	19	5
All	All	766/778 (98%)	743 (97%)	18 (2%)	5 (1%)	26	11

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	14	LYS
1	A	208	ARG
1	B	6	LEU
1	B	12	TYR
1	B	282	GLY

5.3.2 Protein sidechains [i](#)

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	305/319 (96%)	293 (96%)	12 (4%)	39	21
1	B	310/319 (97%)	299 (96%)	11 (4%)	43	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	615/638 (96%)	592 (96%)	23 (4%)	41	23

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	74	LEU
1	A	137	LEU
1	A	138	ARG
1	A	147	LYS
1	A	149	LEU
1	A	163	ARG
1	A	212	LEU
1	A	235	LEU
1	A	277	ARG
1	A	279	LEU
1	A	325	ARG
1	B	6	LEU
1	B	15	ASP
1	B	74	LEU
1	B	153	LEU
1	B	165	MET
1	B	172	LEU
1	B	218	LEU
1	B	280	LEU
1	B	283	GLU
1	B	318	GLU
1	B	365	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	HIS
1	A	300	GLN
1	A	333	GLN
1	A	370	GLN
1	B	67	GLN
1	B	239	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

22 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	SRT	A	601	-	3,9,9	0.73	0	6,12,12	2.10	2 (33%)
3	HEM	A	602	1	24,50,50	2.98	8 (33%)	16,82,82	2.04	7 (43%)
4	EDO	A	705	-	3,3,3	0.55	0	2,2,2	0.47	0
4	EDO	A	713	-	3,3,3	0.41	0	2,2,2	0.43	0
4	EDO	A	714	-	3,3,3	0.36	0	2,2,2	0.45	0
4	EDO	A	715	-	3,3,3	0.52	0	2,2,2	0.31	0
4	EDO	A	717	-	3,3,3	0.49	0	2,2,2	0.31	0
4	EDO	A	718	-	3,3,3	0.47	0	2,2,2	0.58	0
4	EDO	A	719	-	3,3,3	0.39	0	2,2,2	0.77	0
2	SRT	B	602	-	3,9,9	0.29	0	6,12,12	3.03	4 (66%)
3	HEM	B	603	1	24,50,50	2.33	9 (37%)	16,82,82	2.18	7 (43%)
4	EDO	B	701	-	3,3,3	0.77	0	2,2,2	0.20	0
4	EDO	B	702	-	3,3,3	0.84	0	2,2,2	0.34	0
4	EDO	B	703	-	3,3,3	0.30	0	2,2,2	0.59	0
4	EDO	B	704	-	3,3,3	0.64	0	2,2,2	0.05	0
4	EDO	B	706	-	3,3,3	0.43	0	2,2,2	0.34	0
4	EDO	B	707	-	3,3,3	0.73	0	2,2,2	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	B	708	-	3,3,3	0.55	0	2,2,2	0.44	0
4	EDO	B	709	-	3,3,3	0.50	0	2,2,2	0.34	0
4	EDO	B	710	-	3,3,3	0.44	0	2,2,2	0.28	0
4	EDO	B	711	-	3,3,3	0.60	0	2,2,2	0.94	0
4	EDO	B	712	-	3,3,3	0.60	0	2,2,2	0.21	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	SRT	A	601	-	2/2/4/4	0/4/12/12	0/0/0/0
3	HEM	A	602	1	-	0/6/54/54	0/0/8/8
4	EDO	A	705	-	-	0/1/1/1	0/0/0/0
4	EDO	A	713	-	-	0/1/1/1	0/0/0/0
4	EDO	A	714	-	-	0/1/1/1	0/0/0/0
4	EDO	A	715	-	-	0/1/1/1	0/0/0/0
4	EDO	A	717	-	-	0/1/1/1	0/0/0/0
4	EDO	A	718	-	-	0/1/1/1	0/0/0/0
4	EDO	A	719	-	-	0/1/1/1	0/0/0/0
2	SRT	B	602	-	2/2/4/4	0/4/12/12	0/0/0/0
3	HEM	B	603	1	-	0/6/54/54	0/0/8/8
4	EDO	B	701	-	-	0/1/1/1	0/0/0/0
4	EDO	B	702	-	-	0/1/1/1	0/0/0/0
4	EDO	B	703	-	-	0/1/1/1	0/0/0/0
4	EDO	B	704	-	-	0/1/1/1	0/0/0/0
4	EDO	B	706	-	-	0/1/1/1	0/0/0/0
4	EDO	B	707	-	-	0/1/1/1	0/0/0/0
4	EDO	B	708	-	-	0/1/1/1	0/0/0/0
4	EDO	B	709	-	-	0/1/1/1	0/0/0/0
4	EDO	B	710	-	-	0/1/1/1	0/0/0/0
4	EDO	B	711	-	-	0/1/1/1	0/0/0/0
4	EDO	B	712	-	-	0/1/1/1	0/0/0/0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	HEM	C3C-C2C	-6.97	1.31	1.40
3	B	603	HEM	C3C-C2C	-5.64	1.33	1.40
3	A	602	HEM	C3B-C2B	-5.27	1.33	1.40
3	B	603	HEM	C3B-C2B	-4.84	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	HEM	C4D-ND	-2.55	1.33	1.36
3	A	602	HEM	C1D-CHD	-2.07	1.34	1.40
3	B	603	HEM	CMA-C3A	-2.07	1.47	1.51
3	B	603	HEM	C4C-NC	2.19	1.39	1.36
3	A	602	HEM	C3D-C2D	2.57	1.45	1.37
3	B	603	HEM	CAD-C3D	2.61	1.55	1.52
3	A	602	HEM	CAA-C2A	2.66	1.56	1.52
3	B	603	HEM	C3D-C2D	3.08	1.46	1.37
3	B	603	HEM	CMD-C2D	3.32	1.58	1.51
3	A	602	HEM	CMC-C2C	3.90	1.60	1.51
3	B	603	HEM	C1C-NC	4.57	1.42	1.36
3	A	602	HEM	C4C-NC	6.03	1.44	1.36
3	A	602	HEM	C1C-NC	7.57	1.46	1.36

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	SRT	O2-C2-C3	-6.14	91.14	108.67
3	B	603	HEM	CBD-CAD-C3D	-4.00	105.46	112.47
3	A	602	HEM	CAD-CBD-CGD	-3.58	105.81	112.78
3	A	602	HEM	CBD-CAD-C3D	-3.52	106.29	112.47
2	A	601	SRT	O2-C2-C3	-3.31	99.20	108.67
3	A	602	HEM	CMD-C2D-C1D	-2.64	123.82	128.31
3	B	603	HEM	CAD-CBD-CGD	-2.56	107.81	112.78
2	B	602	SRT	C1-C2-C3	-2.46	108.31	113.35
3	B	603	HEM	CMA-C3A-C4A	-2.45	124.15	128.31
3	B	603	HEM	C3B-C4B-NB	-2.19	106.38	109.21
3	A	602	HEM	C3B-C4B-NB	-2.18	106.39	109.21
2	B	602	SRT	C4-C3-C2	2.09	117.63	113.35
2	B	602	SRT	O3-C3-C2	2.15	114.81	108.67
3	A	602	HEM	CMD-C2D-C3D	2.24	129.91	125.24
3	A	602	HEM	CMC-C2C-C3C	2.32	129.62	125.09
3	B	603	HEM	CMC-C2C-C3C	2.33	129.65	125.09
2	A	601	SRT	O3-C3-C4	2.72	117.89	111.12
3	A	602	HEM	CMB-C2B-C3B	3.09	131.13	125.09
3	B	603	HEM	CBA-CAA-C2A	3.22	118.16	112.49
3	B	603	HEM	CMB-C2B-C3B	3.37	131.69	125.09

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	602	SRT	C2

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Mol	Chain	Res	Type	Atom
2	B	602	SRT	C3
2	A	601	SRT	C2
2	A	601	SRT	C3

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	SRT	1	0
3	A	602	HEM	1	0
4	A	714	EDO	1	0
4	A	715	EDO	1	0
4	A	717	EDO	1	0
3	B	603	HEM	1	0
4	B	703	EDO	1	0
4	B	707	EDO	3	0
4	B	708	EDO	1	0
4	B	709	EDO	1	0
4	B	710	EDO	3	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, 95th 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 ²)	Q<0.9
1	A	385/389 (98%)	0.30	24 (6%)	24 19	20, 39, 60, 73	25 (6%)
1	B	382/389 (98%)	0.03	17 (4%)	37 31	15, 27, 55, 82	54 (14%)
All	All	767/778 (98%)	0.16	41 (5%)	30 25	15, 33, 58, 82	79 (10%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	6	LEU	8.8
1	A	40	ARG	7.8
1	A	6	LEU	4.4
1	B	8	GLU	4.3
1	A	41	PHE	4.0
1	A	10	TRP	3.9
1	A	38	LEU	3.8
1	B	15	ASP	3.4
1	A	287	PRO	3.4
1	A	174	LEU	3.3
1	A	30	ALA	3.3
1	B	10	TRP	3.2
1	A	283	GLU	3.1
1	B	37	PRO	3.1
1	B	172	LEU	3.0
1	A	288	PRO	2.9
1	A	382	ARG	2.9
1	A	294	LEU	2.7
1	B	280	LEU	2.6
1	B	278	PRO	2.6
1	A	286	LEU	2.6
1	B	292	LEU	2.5
1	A	289	GLY	2.4
1	A	58	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	205	HIS	2.4
1	B	178	ALA	2.3
1	B	170	SER	2.3
1	B	216	VAL	2.3
1	A	264	LEU	2.3
1	B	7	ARG	2.3
1	B	41	PHE	2.2
1	B	39	PRO	2.2
1	B	294	LEU	2.2
1	A	280	LEU	2.2
1	B	169	ARG	2.1
1	A	46	ILE	2.1
1	A	12	TYR	2.1
1	A	5	SER	2.0
1	A	292	LEU	2.0
1	A	277	ARG	2.0
1	A	285	ARG	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, 95th 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 ²)	Q<0.9
4	EDO	B	709	4/4	0.72	0.43	30.89	55,64,69,71	0
4	EDO	B	707	4/4	0.92	0.33	14.22	40,44,50,50	0
4	EDO	B	708	4/4	0.62	0.46	10.14	60,63,68,68	0
4	EDO	A	717	4/4	0.76	0.36	8.48	62,68,68,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	EDO	B	704	4/4	0.68	0.22	7.61	58,64,67,70	0
2	SRT	B	602	10/10	0.93	0.17	6.08	32,36,41,41	0
2	SRT	A	601	10/10	0.85	0.22	5.18	41,49,55,56	0
4	EDO	A	715	4/4	0.72	0.20	3.95	67,70,70,72	0
4	EDO	B	711	4/4	0.92	0.14	1.68	33,40,43,45	0
4	EDO	B	706	4/4	0.89	0.20	1.65	39,48,49,55	0
4	EDO	B	702	4/4	0.92	0.12	1.31	33,38,39,42	0
4	EDO	B	703	4/4	0.91	0.13	1.25	45,47,50,53	0
4	EDO	B	710	4/4	0.96	0.12	0.54	38,45,46,53	0
4	EDO	A	718	4/4	0.95	0.11	0.53	45,48,50,54	0
4	EDO	A	705	4/4	0.86	0.16	0.40	50,51,54,59	0
4	EDO	A	713	4/4	0.79	0.16	0.12	69,69,69,69	0
4	EDO	B	701	4/4	0.94	0.09	-0.34	33,37,39,41	0
3	HEM	A	602	43/43	0.98	0.06	-1.08	18,24,32,37	0
3	HEM	B	603	43/43	0.99	0.06	-1.45	11,15,24,30	0
4	EDO	A	719	4/4	0.79	0.31	-	58,66,66,71	0
4	EDO	A	714	4/4	0.70	0.25	-	69,70,70,71	0
4	EDO	B	712	4/4	0.86	0.27	-	60,62,62,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.