Full wwPDB X-ray Structure Validation Report (i)

Aug 16, 2016 – 03:58 PM EDT

PDB ID	:	3EJB
Title	:	Crystal Structure of P450BioI in complex with tetradecanoic acid ligated Acyl Carrier Protein
Authors	:	Cryle, M.J.; Schlichting, I.
Deposited on	:	2008-09-18
Resolution	:	2.00 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

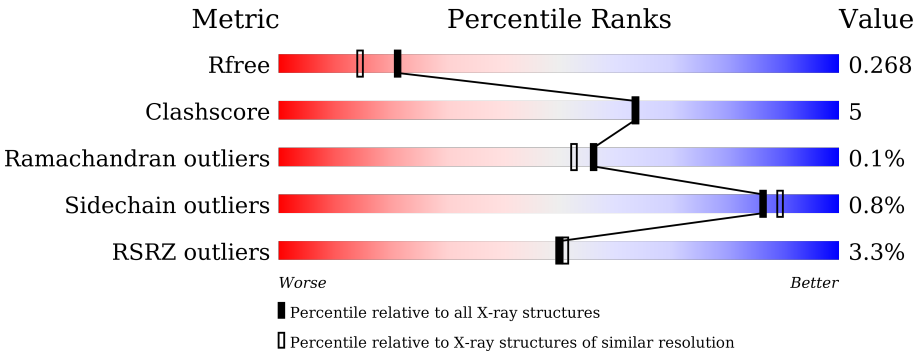
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 <=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	97	5% 72% 8% 20%
1	C	97	3% 74% 5% 21%
1	E	97	5% 70% 10% 20%
1	G	97	% 70% 9% 21%
2	B	404	2% 84% 10% 6%
2	D	404	2% 85% 9%

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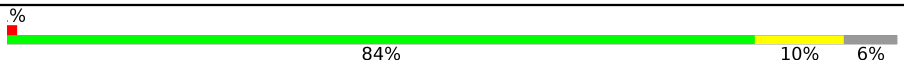
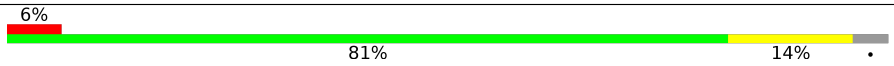
Mol	Chain	Length	Quality of chain
2	F	404	
2	H	404	

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
4	HTG	F	406	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16422 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 Acyl carrier protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	78	Total	C	N	O	S	0	0	0
			606	374	95	135	2			
1	C	77	Total	C	N	O	S	0	0	0
			596	368	92	134	2			
1	E	78	Total	C	N	O	S	0	0	0
			606	374	95	135	2			
1	G	77	Total	C	N	O	S	0	0	0
			596	368	92	134	2			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP P0A6A8
A	2	SER	-	EXPRESSION TAG	UNP P0A6A8
A	3	SER	-	EXPRESSION TAG	UNP P0A6A8
A	4	HIS	-	EXPRESSION TAG	UNP P0A6A8
A	5	HIS	-	EXPRESSION TAG	UNP P0A6A8
A	6	HIS	-	EXPRESSION TAG	UNP P0A6A8
A	7	HIS	-	EXPRESSION TAG	UNP P0A6A8
A	8	HIS	-	EXPRESSION TAG	UNP P0A6A8
A	9	HIS	-	EXPRESSION TAG	UNP P0A6A8
A	10	SER	-	EXPRESSION TAG	UNP P0A6A8
A	11	SER	-	EXPRESSION TAG	UNP P0A6A8
A	12	GLY	-	EXPRESSION TAG	UNP P0A6A8
A	13	LEU	-	EXPRESSION TAG	UNP P0A6A8
A	14	VAL	-	EXPRESSION TAG	UNP P0A6A8
A	15	PRO	-	EXPRESSION TAG	UNP P0A6A8
A	16	ARG	-	EXPRESSION TAG	UNP P0A6A8
A	17	GLY	-	EXPRESSION TAG	UNP P0A6A8
A	18	SER	-	EXPRESSION TAG	UNP P0A6A8
A	19	HIS	-	EXPRESSION TAG	UNP P0A6A8
C	1	GLY	-	EXPRESSION TAG	UNP P0A6A8
C	2	SER	-	EXPRESSION TAG	UNP P0A6A8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	3	SER	-	EXPRESSION TAG	UNP P0A6A8
C	4	HIS	-	EXPRESSION TAG	UNP P0A6A8
C	5	HIS	-	EXPRESSION TAG	UNP P0A6A8
C	6	HIS	-	EXPRESSION TAG	UNP P0A6A8
C	7	HIS	-	EXPRESSION TAG	UNP P0A6A8
C	8	HIS	-	EXPRESSION TAG	UNP P0A6A8
C	9	HIS	-	EXPRESSION TAG	UNP P0A6A8
C	10	SER	-	EXPRESSION TAG	UNP P0A6A8
C	11	SER	-	EXPRESSION TAG	UNP P0A6A8
C	12	GLY	-	EXPRESSION TAG	UNP P0A6A8
C	13	LEU	-	EXPRESSION TAG	UNP P0A6A8
C	14	VAL	-	EXPRESSION TAG	UNP P0A6A8
C	15	PRO	-	EXPRESSION TAG	UNP P0A6A8
C	16	ARG	-	EXPRESSION TAG	UNP P0A6A8
C	17	GLY	-	EXPRESSION TAG	UNP P0A6A8
C	18	SER	-	EXPRESSION TAG	UNP P0A6A8
C	19	HIS	-	EXPRESSION TAG	UNP P0A6A8
E	1	GLY	-	EXPRESSION TAG	UNP P0A6A8
E	2	SER	-	EXPRESSION TAG	UNP P0A6A8
E	3	SER	-	EXPRESSION TAG	UNP P0A6A8
E	4	HIS	-	EXPRESSION TAG	UNP P0A6A8
E	5	HIS	-	EXPRESSION TAG	UNP P0A6A8
E	6	HIS	-	EXPRESSION TAG	UNP P0A6A8
E	7	HIS	-	EXPRESSION TAG	UNP P0A6A8
E	8	HIS	-	EXPRESSION TAG	UNP P0A6A8
E	9	HIS	-	EXPRESSION TAG	UNP P0A6A8
E	10	SER	-	EXPRESSION TAG	UNP P0A6A8
E	11	SER	-	EXPRESSION TAG	UNP P0A6A8
E	12	GLY	-	EXPRESSION TAG	UNP P0A6A8
E	13	LEU	-	EXPRESSION TAG	UNP P0A6A8
E	14	VAL	-	EXPRESSION TAG	UNP P0A6A8
E	15	PRO	-	EXPRESSION TAG	UNP P0A6A8
E	16	ARG	-	EXPRESSION TAG	UNP P0A6A8
E	17	GLY	-	EXPRESSION TAG	UNP P0A6A8
E	18	SER	-	EXPRESSION TAG	UNP P0A6A8
E	19	HIS	-	EXPRESSION TAG	UNP P0A6A8
G	1	GLY	-	EXPRESSION TAG	UNP P0A6A8
G	2	SER	-	EXPRESSION TAG	UNP P0A6A8
G	3	SER	-	EXPRESSION TAG	UNP P0A6A8
G	4	HIS	-	EXPRESSION TAG	UNP P0A6A8
G	5	HIS	-	EXPRESSION TAG	UNP P0A6A8
G	6	HIS	-	EXPRESSION TAG	UNP P0A6A8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	7	HIS	-	EXPRESSION TAG	UNP P0A6A8
G	8	HIS	-	EXPRESSION TAG	UNP P0A6A8
G	9	HIS	-	EXPRESSION TAG	UNP P0A6A8
G	10	SER	-	EXPRESSION TAG	UNP P0A6A8
G	11	SER	-	EXPRESSION TAG	UNP P0A6A8
G	12	GLY	-	EXPRESSION TAG	UNP P0A6A8
G	13	LEU	-	EXPRESSION TAG	UNP P0A6A8
G	14	VAL	-	EXPRESSION TAG	UNP P0A6A8
G	15	PRO	-	EXPRESSION TAG	UNP P0A6A8
G	16	ARG	-	EXPRESSION TAG	UNP P0A6A8
G	17	GLY	-	EXPRESSION TAG	UNP P0A6A8
G	18	SER	-	EXPRESSION TAG	UNP P0A6A8
G	19	HIS	-	EXPRESSION TAG	UNP P0A6A8

- Molecule 2 is a protein called Biotin biosynthesis cytochrome P450-like enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	380	Total	C	N	O	S	0	2	0
			3057	1947	531	565	14			
2	D	386	Total	C	N	O	S	0	1	0
			3097	1968	539	576	14			
2	F	378	Total	C	N	O	S	0	0	0
			3028	1930	525	559	14			
2	H	387	Total	C	N	O	S	0	0	0
			3097	1968	538	577	14			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	395	ALA	-	EXPRESSION TAG	UNP P53554
B	396	SER	-	EXPRESSION TAG	UNP P53554
B	397	TRP	-	EXPRESSION TAG	UNP P53554
B	398	SER	-	EXPRESSION TAG	UNP P53554
B	399	HIS	-	EXPRESSION TAG	UNP P53554
B	400	PRO	-	EXPRESSION TAG	UNP P53554
B	401	GLN	-	EXPRESSION TAG	UNP P53554
B	402	PHE	-	EXPRESSION TAG	UNP P53554
B	403	GLU	-	EXPRESSION TAG	UNP P53554
B	404	LYS	-	EXPRESSION TAG	UNP P53554
D	395	ALA	-	EXPRESSION TAG	UNP P53554
D	396	SER	-	EXPRESSION TAG	UNP P53554
D	397	TRP	-	EXPRESSION TAG	UNP P53554

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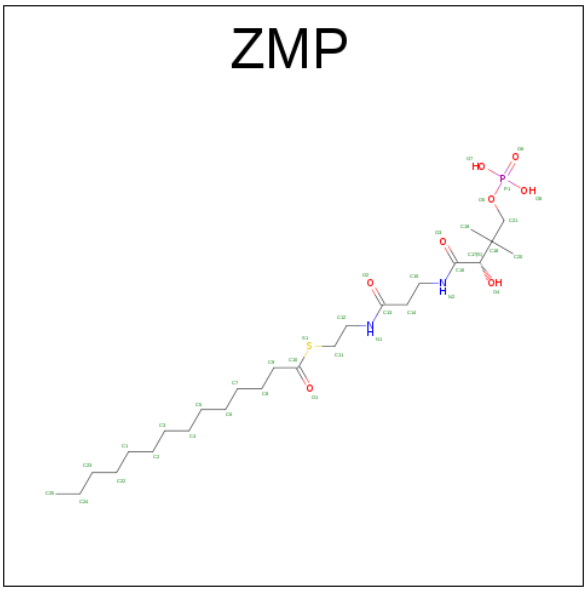
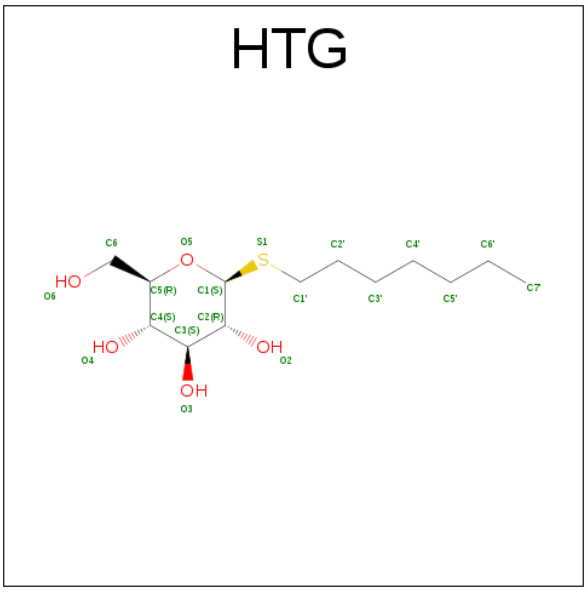
Chain	Residue	Modelled	Actual	Comment	Reference
D	398	SER	-	EXPRESSION TAG	UNP P53554
D	399	HIS	-	EXPRESSION TAG	UNP P53554
D	400	PRO	-	EXPRESSION TAG	UNP P53554
D	401	GLN	-	EXPRESSION TAG	UNP P53554
D	402	PHE	-	EXPRESSION TAG	UNP P53554
D	403	GLU	-	EXPRESSION TAG	UNP P53554
D	404	LYS	-	EXPRESSION TAG	UNP P53554
F	395	ALA	-	EXPRESSION TAG	UNP P53554
F	396	SER	-	EXPRESSION TAG	UNP P53554
F	397	TRP	-	EXPRESSION TAG	UNP P53554
F	398	SER	-	EXPRESSION TAG	UNP P53554
F	399	HIS	-	EXPRESSION TAG	UNP P53554
F	400	PRO	-	EXPRESSION TAG	UNP P53554
F	401	GLN	-	EXPRESSION TAG	UNP P53554
F	402	PHE	-	EXPRESSION TAG	UNP P53554
F	403	GLU	-	EXPRESSION TAG	UNP P53554
F	404	LYS	-	EXPRESSION TAG	UNP P53554
H	395	ALA	-	EXPRESSION TAG	UNP P53554
H	396	SER	-	EXPRESSION TAG	UNP P53554
H	397	TRP	-	EXPRESSION TAG	UNP P53554
H	398	SER	-	EXPRESSION TAG	UNP P53554
H	399	HIS	-	EXPRESSION TAG	UNP P53554
H	400	PRO	-	EXPRESSION TAG	UNP P53554
H	401	GLN	-	EXPRESSION TAG	UNP P53554
H	402	PHE	-	EXPRESSION TAG	UNP P53554
H	403	GLU	-	EXPRESSION TAG	UNP P53554
H	404	LYS	-	EXPRESSION TAG	UNP P53554

- Molecule 3 is S-[2-({N-[(2S)-2-HYDROXY-3,3-DIMETHYL-4-(PHOSPHONOOXY)BUTANOYL]-BETA-ALANYL}AMINO)ETHYL] TETRADECANETHIOATE (three-letter code: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



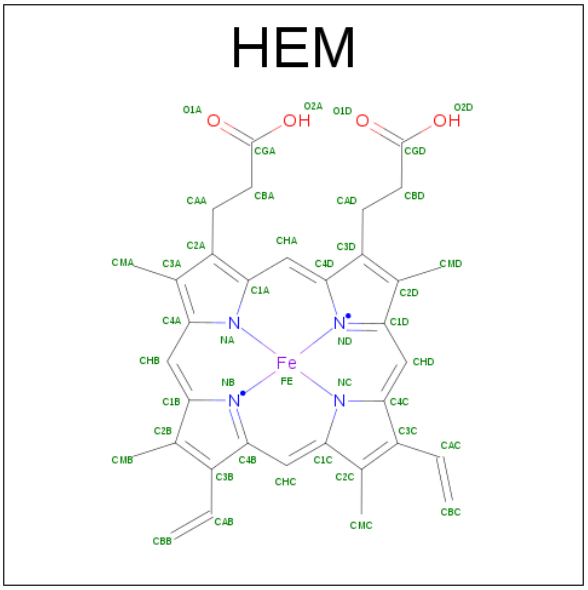
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			36	25	2	7	1	1		
3	C	1	Total	C	N	O	P	S	0	0
			36	25	2	7	1	1		
3	E	1	Total	C	N	O	P	S	0	0
			36	25	2	7	1	1		
3	G	1	Total	C	N	O	P	S	0	0
			36	25	2	7	1	1		

- Molecule 4 is HEPTYL 1-THIOHEXOPYRANOSIDE (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O S 14 8 5 1	0	0
4	A	1	Total C 6 6	0	0
4	C	1	Total C O S 15 9 5 1	0	0
4	D	1	Total C 5 5	0	0
4	E	1	Total C O S 16 10 5 1	0	0
4	F	1	Total C S 5 4 1	0	0
4	G	1	Total C O S 15 9 5 1	0	0
4	H	1	Total C S 7 6 1	0	0

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C Fe N O 43 34 1 4 4	0	0
5	D	1	Total C Fe N O 43 34 1 4 4	0	0
5	F	1	Total C Fe N O 43 34 1 4 4	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		
6	F	1	Total	Cl	0	0
			1	1		

- Molecule 7 is water.

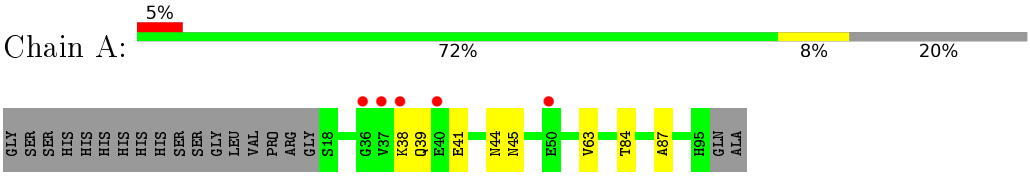
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	78	Total	O	0	0
			78	78		
7	B	290	Total	O	0	0
			290	290		
7	C	67	Total	O	0	0
			67	67		
7	D	241	Total	O	0	0
			241	241		
7	E	81	Total	O	0	0
			81	81		
7	F	289	Total	O	0	0
			289	289		
7	G	78	Total	O	0	0
			78	78		
7	H	214	Total	O	0	0
			214	214		

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.

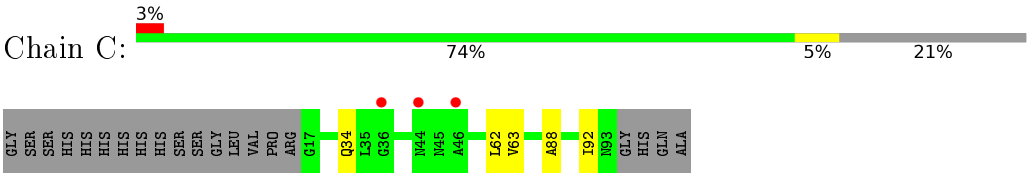
- Molecule 1: Acyl carrier protein

Chain A:



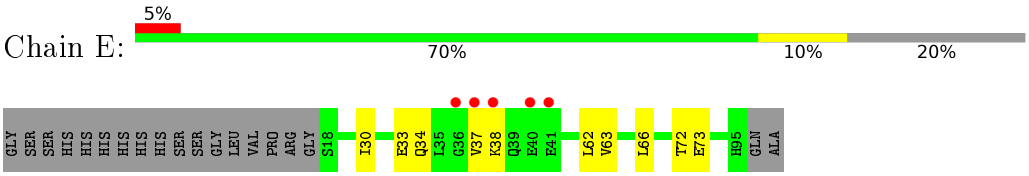
- Molecule 1: Acyl carrier protein

Chain C:



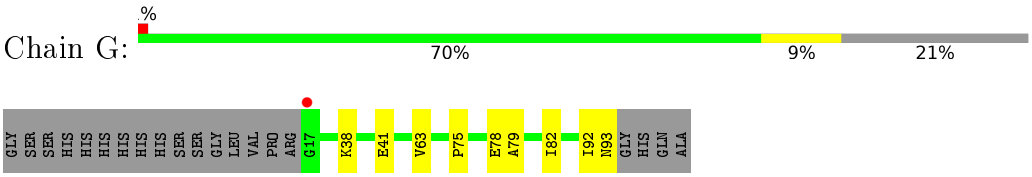
- Molecule 1: Acyl carrier protein

Chain E:



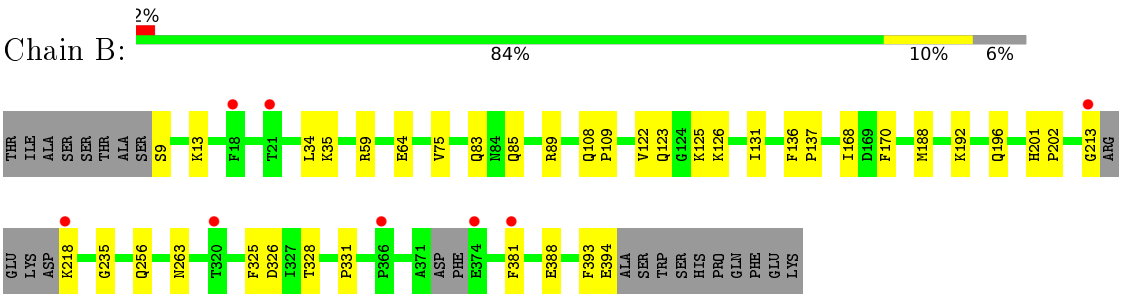
- Molecule 1: Acyl carrier protein

Chain G:



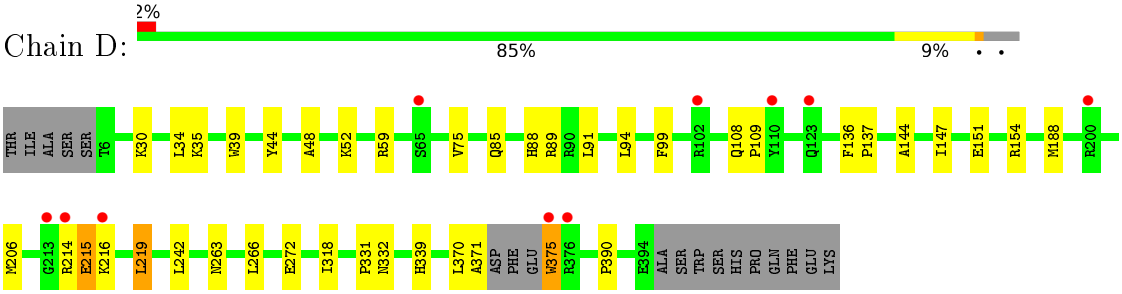
- Molecule 2: Biotin biosynthesis cytochrome P450-like enzyme

Chain B:



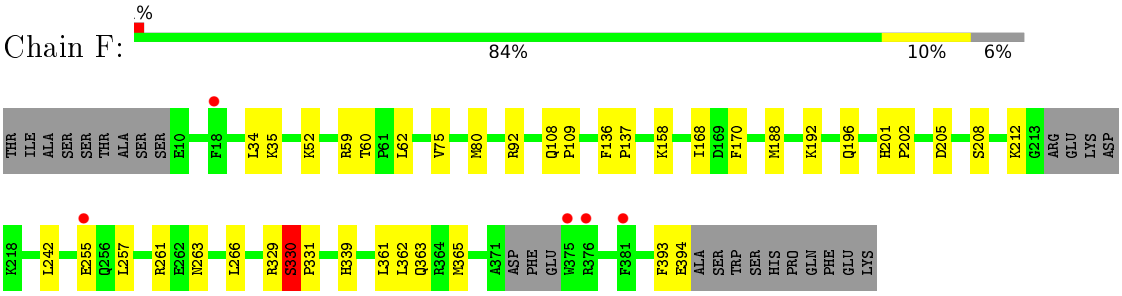
• Molecule 2: Biotin biosynthesis cytochrome P450-like enzyme

Chain D:



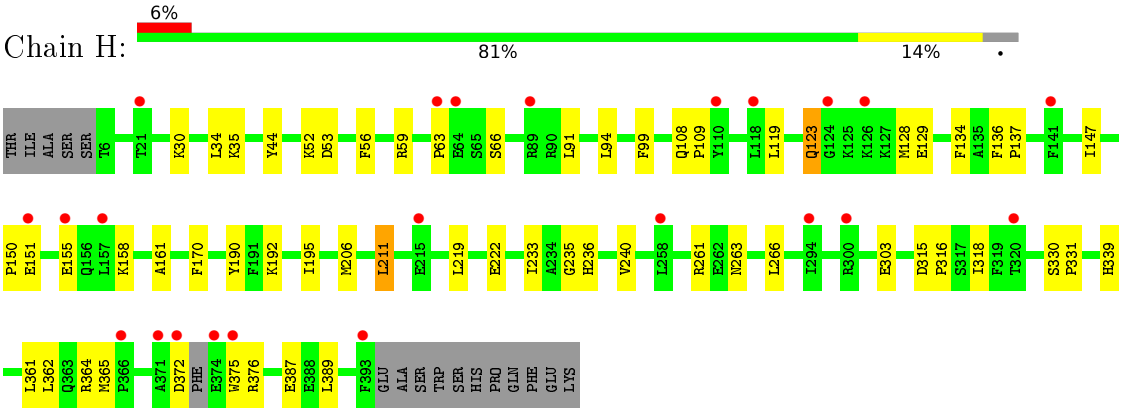
• Molecule 2: Biotin biosynthesis cytochrome P450-like enzyme

Chain F:



• Molecule 2: Biotin biosynthesis cytochrome P450-like enzyme

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	61.30Å 92.10Å 107.70Å 109.00° 89.20° 90.10°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.7 (20.00-2.00) 84.5 (20.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	6.00 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.222 , 0.266 0.223 , 0.268	Depositor DCC
R_{free} test set	7336 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	26.4	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 30.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.157 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16422	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: HTG, HEM, ZMP, CL

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	0.21	0/611	0.35	0/826
1	C	0.23	0/600	0.34	0/811
1	E	0.21	0/611	0.34	0/826
1	G	0.23	0/600	0.34	0/811
2	B	0.22	0/3129	0.35	0/4239
2	D	0.22	0/3164	0.35	0/4289
2	F	0.23	0/3094	0.35	0/4193
2	H	0.22	0/3164	0.35	0/4288
All	All	0.22	0/14973	0.35	0/20283

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
2	F	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	329	ARG	Peptide
2	F	330	SER	Peptide

5.2 Too-close contacts (i)

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	606	0	578	5	0
1	C	596	0	571	3	0
1	E	606	0	578	5	0
1	G	596	0	571	6	0
2	B	3057	0	3064	26	0
2	D	3097	0	3097	32	0
2	F	3028	0	3032	35	1
2	H	3097	0	3095	41	1
3	A	36	0	45	2	0
3	C	36	0	45	2	0
3	E	36	0	45	4	0
3	G	36	0	45	2	0
4	A	20	0	24	0	0
4	C	15	0	15	0	0
4	D	5	0	9	0	0
4	E	16	0	17	0	0
4	F	5	0	6	1	0
4	G	15	0	15	0	0
4	H	7	0	10	0	0
5	B	43	0	30	1	0
5	D	43	0	30	1	0
5	F	43	0	30	1	0
5	H	43	0	30	1	0
6	B	1	0	0	0	0
6	F	1	0	0	1	0
7	A	78	0	0	2	0
7	B	290	0	0	4	0
7	C	67	0	0	0	0
7	D	241	0	0	2	0
7	E	81	0	0	0	0
7	F	289	0	0	6	0
7	G	78	0	0	0	0
7	H	214	0	0	1	0
All	All	16422	0	14982	157	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (157) 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)
2:F:330:SER:HB2	2:F:331:PRO:HD2	1.34	1.07
2:D:94:LEU:HD13	2:D:219:LEU:HD13	1.44	0.98
2:H:375:TRP:HE1	2:H:389:LEU:HD12	1.30	0.96
2:H:263:ASN:ND2	2:H:266:LEU:HG	1.87	0.90
1:G:92:ILE:O	1:G:93:ASN:HB2	1.75	0.87
2:F:330:SER:CB	2:F:331:PRO:HD2	2.09	0.83
2:F:330:SER:HB2	2:F:331:PRO:CD	2.08	0.81
2:H:94:LEU:HD13	2:H:219:LEU:HG	1.62	0.81
3:G:99:ZMP:O3	3:G:99:ZMP:H20A	1.80	0.80
2:F:52:LYS:HE3	2:F:339:HIS:NE2	1.97	0.80
2:H:136:PHE:HZ	2:H:158:LYS:HB2	1.47	0.80
2:F:80:MET:SD	7:F:567:HOH:O	2.39	0.78
2:D:91:LEU:HD23	2:D:219:LEU:HD11	1.67	0.77
2:B:123:GLN:NE2	2:B:394:GLU:OE2	2.17	0.76
2:B:331:PRO:O	7:B:457:HOH:O	2.03	0.76
2:H:123:GLN:HG3	2:H:364:ARG:HH21	1.52	0.75
2:F:80:MET:HE3	2:F:92:ARG:HB2	1.66	0.75
1:E:63:VAL:HG11	2:F:35:LYS:HE2	1.68	0.73
2:F:330:SER:CB	2:F:331:PRO:CD	2.65	0.71
2:H:372:ASP:H	2:H:375:TRP:HH2	1.38	0.71
2:H:361:LEU:HD12	2:H:365:MET:HE3	1.73	0.71
2:B:326:ASP:OD1	2:B:328:THR:HG22	1.91	0.70
2:D:331:PRO:O	7:D:615:HOH:O	2.10	0.69
2:H:128:MET:HE1	2:H:134:PHE:HB2	1.75	0.69
2:D:94:LEU:CD1	2:D:219:LEU:HD13	2.22	0.68
2:D:151:GLU:HA	2:D:154:ARG:HE	1.57	0.68
2:F:34:LEU:HD12	2:F:170:PHE:HB3	1.75	0.68
2:D:48:ALA:O	2:D:52:LYS:HG3	1.94	0.67
2:H:331:PRO:O	7:H:492:HOH:O	2.12	0.67
2:D:263:ASN:ND2	7:D:493:HOH:O	2.26	0.67
2:D:85:GLN:OE1	2:D:89:ARG:HG2	1.96	0.66
2:B:192:LYS:O	2:B:196:GLN:HG2	1.97	0.65
2:F:331:PRO:O	7:F:475:HOH:O	2.14	0.65
2:B:34:LEU:HD12	2:B:170:PHE:HB3	1.79	0.65
2:F:205:ASP:HA	4:F:406:HTG:H2'2	1.78	0.64
3:G:99:ZMP:O3	3:G:99:ZMP:C20	2.46	0.63
3:E:99:ZMP:C19	3:E:99:ZMP:O3	2.46	0.63
2:F:263:ASN:ND2	7:F:577:HOH:O	2.33	0.62
1:C:63:VAL:HG11	2:D:35:LYS:HE2	1.80	0.62
3:E:99:ZMP:H19	3:E:99:ZMP:O3	1.98	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:99:ZMP:O3	3:A:99:ZMP:C19	2.50	0.59
2:B:89[A]:ARG:HG2	7:B:424:HOH:O	2.03	0.59
2:F:263:ASN:OD1	2:F:266:LEU:HG	2.03	0.58
2:H:136:PHE:CZ	2:H:158:LYS:HB2	2.35	0.58
3:E:99:ZMP:H6A	3:E:99:ZMP:H2A	1.86	0.58
2:F:242:LEU:HD22	5:F:405:HEM:HBB1	1.85	0.58
2:H:195:ILE:HG23	2:H:211:LEU:HD21	1.85	0.58
2:H:375:TRP:NE1	2:H:389:LEU:HD12	2.11	0.58
1:G:92:ILE:O	1:G:93:ASN:CB	2.51	0.57
2:H:136:PHE:HZ	2:H:158:LYS:CB	2.17	0.57
2:H:136:PHE:HB3	2:H:137:PRO:HD3	1.86	0.57
2:D:242:LEU:HD22	5:D:405:HEM:HBB1	1.86	0.57
3:A:99:ZMP:O3	3:A:99:ZMP:H19	2.03	0.57
2:H:52:LYS:HE3	2:H:339:HIS:NE2	2.20	0.57
2:D:151:GLU:HA	2:D:154:ARG:NE	2.20	0.57
1:A:63:VAL:HG11	2:B:35:LYS:HE2	1.87	0.56
2:H:34:LEU:HD22	2:H:170:PHE:HB3	1.87	0.56
2:B:136:PHE:HB3	2:B:137:PRO:HD3	1.87	0.56
2:F:261:ARG:NH1	2:F:362:LEU:O	2.39	0.55
1:E:33:GLU:HG2	1:E:38:LYS:HE2	1.87	0.55
1:G:63:VAL:HG11	2:H:35:LYS:HE2	1.88	0.55
2:F:192:LYS:O	2:F:196:GLN:HG2	2.06	0.54
2:H:147:ILE:HA	2:H:206:MET:HB3	1.90	0.54
2:D:99:PHE:CE2	2:D:206:MET:HE1	2.44	0.53
2:F:60:THR:OG1	7:F:538:HOH:O	2.19	0.52
1:C:34:GLN:HG2	1:C:62:LEU:CD2	2.40	0.52
2:F:363:GLN:HG3	7:F:625:HOH:O	2.09	0.52
1:A:84:THR:HG23	1:A:87:ALA:H	1.75	0.52
2:H:91:LEU:HD23	2:H:219:LEU:HD21	1.92	0.52
1:G:79:ALA:O	1:G:82:ILE:HG12	2.09	0.51
1:A:44:ASN:O	1:A:45:ASN:HB2	2.09	0.51
2:D:144:ALA:HB3	2:D:154:ARG:HH11	1.75	0.51
2:B:263:ASN:OD1	2:D:263:ASN:OD1	2.30	0.50
2:D:370:LEU:HD13	2:D:375:TRP:CZ3	2.47	0.50
3:C:99:ZMP:H19	3:C:99:ZMP:O3	2.11	0.50
2:F:208:SER:O	2:F:212:LYS:HG2	2.11	0.50
3:C:99:ZMP:C19	3:C:99:ZMP:O3	2.59	0.50
2:F:80:MET:HE3	2:F:92:ARG:CB	2.41	0.50
2:D:147:ILE:HA	2:D:206:MET:HB3	1.94	0.50
2:D:85:GLN:NE2	2:D:89:ARG:NH1	2.59	0.50
2:F:136:PHE:HB3	2:F:137:PRO:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:GLN:C	1:A:41:GLU:H	2.16	0.49
2:D:272:GLU:HB3	2:D:332[B]:ASN:OD1	2.12	0.49
2:H:53:ASP:HB3	2:H:56:PHE:HD2	1.77	0.49
2:H:119:LEU:HD13	2:H:365:MET:HE1	1.93	0.49
2:B:75:VAL:HG22	2:B:188:MET:HE3	1.94	0.49
2:B:131:ILE:HD12	2:B:388:GLU:HA	1.94	0.49
2:D:85:GLN:HE22	2:D:88:HIS:HB3	1.76	0.49
2:F:60:THR:HG23	2:F:62:LEU:O	2.13	0.49
2:F:80:MET:CE	2:F:92:ARG:HB2	2.39	0.49
2:B:256:GLN:NE2	2:B:325:PHE:O	2.29	0.48
7:A:119:HOH:O	2:B:64:GLU:HG3	2.13	0.48
2:F:75:VAL:HG22	2:F:188:MET:HE3	1.94	0.48
2:B:122:VAL:HA	2:B:125:LYS:HD2	1.95	0.48
2:D:215:GLU:HB3	2:D:216:LYS:H	1.42	0.48
2:D:263:ASN:OD1	2:D:266:LEU:HG	2.13	0.47
2:H:108:GLN:HB3	2:H:109:PRO:HD3	1.96	0.47
2:D:75:VAL:HG22	2:D:188:MET:HE3	1.96	0.47
2:F:108:GLN:HB3	2:F:109:PRO:HD3	1.97	0.47
2:B:34:LEU:O	2:B:35:LYS:HB2	2.14	0.46
2:D:136:PHE:HB3	2:D:137:PRO:HD3	1.97	0.46
2:D:108:GLN:HB3	2:D:109:PRO:HD3	1.97	0.46
2:F:34:LEU:O	2:F:35:LYS:HB2	2.14	0.46
2:H:155:GLU:O	2:H:158:LYS:HG2	2.16	0.46
2:D:52:LYS:HE2	2:D:339:HIS:NE2	2.32	0.45
2:F:393:PHE:HD1	2:F:394:GLU:HG2	1.81	0.45
2:H:376:ARG:HG2	2:H:387:GLU:HG3	1.98	0.45
1:C:88:ALA:O	1:C:92:ILE:HG12	2.17	0.45
2:H:330:SER:HA	2:H:331:PRO:HA	1.80	0.45
2:H:123:GLN:HG3	2:H:364:ARG:NH2	2.26	0.45
1:E:30:ILE:HD12	1:E:66:LEU:HD23	1.99	0.45
2:F:255:GLU:HB2	6:F:407:CL:CL	2.54	0.44
2:H:236:HIS:O	2:H:240:VAL:HG23	2.17	0.44
2:B:9:SER:O	2:B:13:LYS:HG3	2.18	0.44
2:H:99:PHE:CE2	2:H:206:MET:HE1	2.52	0.44
2:B:89[B]:ARG:HA	2:B:89[B]:ARG:HD3	1.86	0.43
2:H:52:LYS:HG3	2:H:339:HIS:CD2	2.52	0.43
2:H:192:LYS:HE2	2:H:222:GLU:HG2	2.01	0.43
2:B:381:PHE:HB3	7:B:683:HOH:O	2.17	0.43
2:D:34:LEU:O	2:D:35:LYS:HB2	2.18	0.43
2:H:44:TYR:CG	2:H:318:ILE:HG13	2.53	0.43
2:B:213:GLY:HA3	2:B:218:LYS:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:75:PRO:HG2	1:G:78:GLU:HB2	2.01	0.43
2:F:363:GLN:HB3	7:F:685:HOH:O	2.18	0.43
2:B:235:GLY:HA2	5:B:405:HEM:CBB	2.49	0.42
2:D:44:TYR:CG	2:D:318:ILE:HG13	2.55	0.42
1:G:38:LYS:O	1:G:41:GLU:HG2	2.19	0.42
2:H:263:ASN:HD22	2:H:266:LEU:HG	1.75	0.42
2:H:235:GLY:HA2	5:H:405:HEM:HAB	2.02	0.42
2:B:126:LYS:HG3	2:B:393:PHE:O	2.19	0.42
2:H:91:LEU:HD23	2:H:219:LEU:CD2	2.50	0.42
3:E:99:ZMP:H24	2:F:168:ILE:HD13	2.01	0.41
2:H:63:PRO:HB2	2:H:66:SER:HB2	2.01	0.41
2:F:201:HIS:HA	2:F:202:PRO:HD2	1.93	0.41
2:D:332[B]:ASN:CG	2:D:332[B]:ASN:O	2.58	0.41
1:E:72:THR:HG22	1:E:73:GLU:N	2.35	0.41
2:H:30:LYS:NZ	2:H:303:GLU:OE2	2.53	0.41
2:H:261:ARG:NH1	2:H:362:LEU:O	2.54	0.41
2:F:394:GLU:OE1	2:F:394:GLU:HA	2.20	0.41
2:D:30:LYS:HD3	2:D:39:TRP:CE2	2.55	0.41
2:F:136:PHE:CZ	2:F:158:LYS:HG3	2.55	0.41
2:F:257:LEU:HD21	2:F:261:ARG:HH21	1.86	0.41
1:E:34:GLN:HG2	1:E:62:LEU:HG	2.03	0.41
2:F:361:LEU:O	2:F:365:MET:HG2	2.20	0.41
2:B:108:GLN:N	2:B:109:PRO:CD	2.84	0.41
2:D:30:LYS:HB2	2:D:39:TRP:CZ3	2.56	0.41
2:B:201:HIS:HA	2:B:202:PRO:HD2	1.96	0.41
2:H:315:ASP:HA	2:H:316:PRO:HD3	1.84	0.41
1:A:38:LYS:HB3	1:A:38:LYS:HE2	1.82	0.40
2:B:85:GLN:HA	7:B:424:HOH:O	2.22	0.40
2:H:150:PRO:HD2	2:H:190:TYR:OH	2.21	0.40
7:A:177:HOH:O	2:B:168:ILE:HB	2.20	0.40
2:H:161:ALA:HA	2:H:233:ILE:HG12	2.03	0.40
2:B:108:GLN:HB3	2:B:109:PRO:HD3	2.04	0.40
2:D:371:ALA:HB3	2:D:390:PRO:HB2	2.02	0.40
2:D:85:GLN:NE2	2:D:88:HIS:HB3	2.36	0.40
2:H:151:GLU:CD	2:H:151:GLU:H	2.24	0.40

All (1) 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)
2:F:263:ASN:OD1	2:H:263:ASN:ND2[1_544]	1.99	0.21

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	76/97 (78%)	73 (96%)	3 (4%)	0	100	100
1	C	75/97 (77%)	75 (100%)	0	0	100	100
1	E	76/97 (78%)	73 (96%)	3 (4%)	0	100	100
1	G	75/97 (77%)	75 (100%)	0	0	100	100
2	B	376/404 (93%)	368 (98%)	8 (2%)	0	100	100
2	D	383/404 (95%)	367 (96%)	16 (4%)	0	100	100
2	F	372/404 (92%)	364 (98%)	7 (2%)	1 (0%)	46	41
2	H	383/404 (95%)	367 (96%)	16 (4%)	0	100	100
All	All	1816/2004 (91%)	1762 (97%)	53 (3%)	1 (0%)	56	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	330	SER

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	68/83 (82%)	68 (100%)	0	100	100
1	C	67/83 (81%)	67 (100%)	0	100	100
1	E	68/83 (82%)	67 (98%)	1 (2%)	72	75
1	G	67/83 (81%)	67 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	336/355 (95%)	334 (99%)	2 (1%)	90 93
2	D	340/355 (96%)	335 (98%)	5 (2%)	72 75
2	F	332/355 (94%)	331 (100%)	1 (0%)	94 96
2	H	340/355 (96%)	336 (99%)	4 (1%)	78 81
All	All	1618/1752 (92%)	1605 (99%)	13 (1%)	86 89

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	59	ARG
2	B	83	GLN
2	D	59	ARG
2	D	214	ARG
2	D	215	GLU
2	D	219	LEU
2	D	375	TRP
1	E	37	VAL
2	F	59	ARG
2	H	59	ARG
2	H	123	GLN
2	H	129	GLU
2	H	211	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	201	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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 for Mogul analysis.

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	$\#\|Z\| > 2$
4	HTG	A	100	-	14,14,19	2.47	2 (14%)	17,19,24	0.70	0
4	HTG	A	101	-	5,5,19	0.50	0	4,4,24	0.54	0
3	ZMP	A	99	1	28,35,36	2.26	6 (21%)	33,42,45	2.24	8 (24%)
5	HEM	B	405	2	24,50,50	2.31	7 (29%)	16,82,82	1.51	2 (12%)
4	HTG	C	100	-	15,15,19	3.57	2 (13%)	18,20,24	1.61	1 (5%)
3	ZMP	C	99	1	28,35,36	2.27	6 (21%)	33,42,45	2.24	8 (24%)
5	HEM	D	405	2	24,50,50	2.34	7 (29%)	16,82,82	1.51	3 (18%)
4	HTG	D	406	-	4,4,19	0.44	0	3,3,24	0.55	0
4	HTG	E	100	-	16,16,19	3.44	2 (12%)	19,21,24	1.67	1 (5%)
3	ZMP	E	99	1	28,35,36	2.27	6 (21%)	33,42,45	2.26	8 (24%)
5	HEM	F	405	2	24,50,50	2.33	6 (25%)	16,82,82	1.58	3 (18%)
4	HTG	F	406	-	4,4,19	2.08	1 (25%)	3,3,24	0.83	0
4	HTG	G	100	-	15,15,19	3.56	2 (13%)	18,20,24	1.76	1 (5%)
3	ZMP	G	99	1	28,35,36	2.28	6 (21%)	33,42,45	2.18	7 (21%)
5	HEM	H	405	2	24,50,50	2.35	7 (29%)	16,82,82	1.56	2 (12%)
4	HTG	H	406	-	6,6,19	1.76	1 (16%)	4,5,24	0.87	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
4	HTG	A	100	-	-	0/5/25/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HTG	A	101	-	-	0/3/3/30	0/0/0/1
3	ZMP	A	99	1	-	0/40/42/43	0/0/0/0
5	HEM	B	405	2	-	0/6/54/54	0/0/8/8
4	HTG	C	100	-	-	0/6/26/30	0/1/1/1
3	ZMP	C	99	1	-	0/40/42/43	0/0/0/0
5	HEM	D	405	2	-	0/6/54/54	0/0/8/8
4	HTG	D	406	-	-	0/2/2/30	0/0/0/1
4	HTG	E	100	-	-	0/7/27/30	0/1/1/1
3	ZMP	E	99	1	-	0/40/42/43	0/0/0/0
5	HEM	F	405	2	-	0/6/54/54	0/0/8/8
4	HTG	F	406	-	-	0/2/2/30	0/0/0/1
4	HTG	G	100	-	-	0/6/26/30	0/1/1/1
3	ZMP	G	99	1	-	0/40/42/43	0/0/0/0
5	HEM	H	405	2	-	0/6/54/54	0/0/8/8
4	HTG	H	406	-	-	0/4/4/30	0/0/0/1

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	100	HTG	C1'-S1	-10.79	1.66	1.81
4	G	100	HTG	C1'-S1	-10.78	1.66	1.81
4	C	100	HTG	C1'-S1	-10.76	1.66	1.81
4	C	100	HTG	C1-S1	-8.62	1.67	1.80
4	G	100	HTG	C1-S1	-8.55	1.67	1.80
4	A	100	HTG	C1-S1	-8.42	1.67	1.80
4	E	100	HTG	C1-S1	-8.40	1.67	1.80
5	F	405	HEM	C3C-C2C	-5.04	1.34	1.40
5	H	405	HEM	C3B-C2B	-4.99	1.34	1.40
5	D	405	HEM	C3C-C2C	-4.91	1.34	1.40
5	H	405	HEM	C3C-C2C	-4.78	1.34	1.40
5	B	405	HEM	C3C-C2C	-4.75	1.34	1.40
5	D	405	HEM	C3B-C2B	-4.71	1.34	1.40
5	B	405	HEM	C3B-C2B	-4.62	1.34	1.40
5	F	405	HEM	C3B-C2B	-4.61	1.34	1.40
4	H	406	HTG	C1'-S1	-4.09	1.66	1.80
4	F	406	HTG	C1'-S1	-4.06	1.66	1.80
4	A	100	HTG	C1'-S1	-3.62	1.66	1.81
3	G	99	ZMP	C16-N2	-3.57	1.26	1.33
3	C	99	ZMP	C16-N2	-3.47	1.26	1.33
3	E	99	ZMP	C16-N2	-3.46	1.26	1.33
3	A	99	ZMP	C16-N2	-3.34	1.26	1.33
3	G	99	ZMP	C13-N1	-2.83	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	99	ZMP	C13-N1	-2.80	1.26	1.33
3	C	99	ZMP	C13-N1	-2.80	1.26	1.33
3	E	99	ZMP	C13-N1	-2.75	1.26	1.33
5	D	405	HEM	CAD-C3D	2.05	1.54	1.52
5	B	405	HEM	CAD-C3D	2.11	1.55	1.52
5	H	405	HEM	CAD-C3D	2.15	1.55	1.52
5	D	405	HEM	C4D-ND	2.37	1.39	1.36
3	E	99	ZMP	C9-C10	2.37	1.52	1.50
3	G	99	ZMP	C9-C10	2.37	1.52	1.50
5	B	405	HEM	C4D-ND	2.44	1.40	1.36
5	F	405	HEM	C4D-ND	2.45	1.40	1.36
5	H	405	HEM	C4D-ND	2.47	1.40	1.36
3	C	99	ZMP	C9-C10	2.63	1.53	1.50
3	A	99	ZMP	C9-C10	2.85	1.53	1.50
5	H	405	HEM	C3B-CAB	3.26	1.54	1.47
5	B	405	HEM	C3B-CAB	3.34	1.54	1.47
5	H	405	HEM	C3C-CAC	3.37	1.54	1.47
5	F	405	HEM	C3C-CAC	3.39	1.54	1.47
5	B	405	HEM	C3C-CAC	3.40	1.54	1.47
5	D	405	HEM	C3C-CAC	3.42	1.54	1.47
5	D	405	HEM	C3B-CAB	3.43	1.55	1.47
5	F	405	HEM	C3B-CAB	3.44	1.55	1.47
3	C	99	ZMP	O2-C13	4.81	1.33	1.23
3	E	99	ZMP	O2-C13	4.85	1.33	1.23
3	A	99	ZMP	O2-C13	4.86	1.33	1.23
3	G	99	ZMP	O2-C13	4.89	1.33	1.23
3	C	99	ZMP	O3-C16	5.24	1.33	1.23
5	D	405	HEM	C3D-C2D	5.26	1.53	1.37
3	A	99	ZMP	O3-C16	5.28	1.33	1.23
5	F	405	HEM	C3D-C2D	5.28	1.53	1.37
3	G	99	ZMP	O3-C16	5.30	1.33	1.23
5	B	405	HEM	C3D-C2D	5.32	1.53	1.37
5	H	405	HEM	C3D-C2D	5.34	1.53	1.37
3	E	99	ZMP	O3-C16	5.35	1.33	1.23
3	A	99	ZMP	O1-C10	7.86	1.33	1.21
3	G	99	ZMP	O1-C10	7.98	1.33	1.21
3	C	99	ZMP	O1-C10	8.01	1.33	1.21
3	E	99	ZMP	O1-C10	8.03	1.33	1.21

All (44) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	99	ZMP	O1-C10-C9	-6.50	119.46	123.94
3	E	99	ZMP	O1-C10-C9	-6.46	119.50	123.94
3	C	99	ZMP	O1-C10-C9	-5.70	120.02	123.94
3	G	99	ZMP	O1-C10-C9	-5.69	120.02	123.94
3	E	99	ZMP	O1-C10-S1	-4.54	119.23	122.83
3	C	99	ZMP	O1-C10-S1	-4.51	119.26	122.83
3	G	99	ZMP	O1-C10-S1	-3.99	119.67	122.83
3	C	99	ZMP	C11-C12-N1	-3.62	105.16	112.43
3	A	99	ZMP	O1-C10-S1	-3.56	120.01	122.83
3	G	99	ZMP	C14-C15-N2	-3.47	104.17	111.94
5	H	405	HEM	C3B-CAB-CBB	-3.39	119.58	126.40
3	G	99	ZMP	C11-C12-N1	-3.29	105.82	112.43
3	E	99	ZMP	C11-C12-N1	-3.25	105.90	112.43
3	E	99	ZMP	C14-C15-N2	-3.25	104.67	111.94
5	F	405	HEM	C3C-CAC-CBC	-3.24	119.88	126.40
5	D	405	HEM	C3C-CAC-CBC	-3.18	120.01	126.40
5	B	405	HEM	C3C-CAC-CBC	-3.04	120.29	126.40
5	H	405	HEM	C3C-CAC-CBC	-3.04	120.29	126.40
5	F	405	HEM	C3B-CAB-CBB	-2.96	120.44	126.40
3	C	99	ZMP	C14-C15-N2	-2.90	105.45	111.94
3	A	99	ZMP	C11-C12-N1	-2.89	106.62	112.43
5	D	405	HEM	C3B-CAB-CBB	-2.85	120.66	126.40
5	B	405	HEM	C3B-CAB-CBB	-2.78	120.81	126.40
3	A	99	ZMP	C14-C15-N2	-2.62	106.08	111.94
5	F	405	HEM	CBD-CAD-C3D	-2.49	108.11	112.47
5	D	405	HEM	CBD-CAD-C3D	-2.17	108.66	112.47
3	C	99	ZMP	C14-C13-N1	2.00	119.94	116.46
3	E	99	ZMP	C11-S1-C10	2.01	109.26	102.09
3	G	99	ZMP	C12-N1-C13	2.14	127.05	122.79
3	A	99	ZMP	C12-N1-C13	2.24	127.23	122.79
3	E	99	ZMP	C12-N1-C13	2.26	127.28	122.79
3	C	99	ZMP	C12-N1-C13	2.28	127.32	122.79
3	C	99	ZMP	C15-N2-C16	2.47	127.56	122.62
3	G	99	ZMP	C15-N2-C16	2.52	127.67	122.62
3	E	99	ZMP	C15-N2-C16	2.62	127.87	122.62
3	A	99	ZMP	C11-S1-C10	2.71	111.74	102.09
3	A	99	ZMP	C15-N2-C16	3.09	128.81	122.62
4	C	100	HTG	C1'-S1-C1	6.21	108.58	100.60
4	E	100	HTG	C1'-S1-C1	6.66	109.16	100.60
3	E	99	ZMP	C9-C10-S1	6.86	119.53	113.36
4	G	100	HTG	C1'-S1-C1	6.88	109.44	100.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	99	ZMP	C9-C10-S1	6.91	119.57	113.36
3	C	99	ZMP	C9-C10-S1	7.33	119.95	113.36
3	A	99	ZMP	C9-C10-S1	7.44	120.05	113.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	99	ZMP	2	0
5	B	405	HEM	1	0
3	C	99	ZMP	2	0
5	D	405	HEM	1	0
3	E	99	ZMP	4	0
5	F	405	HEM	1	0
4	F	406	HTG	1	0
3	G	99	ZMP	2	0
5	H	405	HEM	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

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^{th} 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	78/97 (80%)	0.32	5 (6%)	23	24	20, 32, 47, 49	0
1	C	77/97 (79%)	0.51	3 (3%)	43	45	21, 36, 43, 44	0
1	E	78/97 (80%)	0.43	5 (6%)	23	24	20, 31, 44, 47	0
1	G	77/97 (79%)	0.22	1 (1%)	79	80	20, 29, 37, 38	0
2	B	380/404 (94%)	0.09	8 (2%)	67	67	15, 24, 35, 42	0
2	D	386/404 (95%)	0.20	10 (2%)	59	60	13, 26, 42, 49	0
2	F	378/404 (93%)	0.09	5 (1%)	79	80	15, 25, 35, 38	0
2	H	387/404 (95%)	0.45	23 (5%)	26	27	17, 31, 43, 51	1 (0%)
All	All	1841/2004 (91%)	0.24	60 (3%)	50	51	13, 28, 41, 51	1 (0%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	375	TRP	6.9
1	G	17	GLY	5.1
1	E	41	GLU	4.9
2	F	381	PHE	4.8
1	E	37	VAL	4.8
2	H	124	GLY	4.6
2	D	213	GLY	4.4
2	B	381	PHE	4.2
2	D	214	ARG	4.2
2	D	110	TYR	4.0
2	H	63	PRO	3.8
2	H	294	ILE	3.7
2	F	18	PHE	3.6
2	D	123	GLN	3.5
1	E	40	GLU	3.4
2	F	255	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
2	H	126	LYS	3.4
2	H	372	ASP	3.3
1	E	38	LYS	3.3
2	H	320	THR	3.2
2	H	141	PHE	3.0
2	B	320	THR	2.9
2	H	371	ALA	2.9
2	H	366	PRO	2.9
2	H	21	THR	2.9
2	H	215	GLU	2.9
2	D	216	LYS	2.7
2	H	374	GLU	2.7
1	A	38	LYS	2.7
2	B	18	PHE	2.6
2	F	375	TRP	2.5
2	H	157	LEU	2.5
2	B	213	GLY	2.5
2	D	65	SER	2.4
1	A	36	GLY	2.4
2	H	110	TYR	2.4
1	A	37	VAL	2.4
1	C	46	ALA	2.3
2	D	375	TRP	2.3
1	C	44	ASN	2.3
2	D	200	ARG	2.3
2	B	374	GLU	2.3
2	H	89	ARG	2.3
2	H	258	LEU	2.2
1	A	40	GLU	2.2
1	A	50	GLU	2.2
2	F	376	ARG	2.2
2	H	155	GLU	2.2
2	D	102	ARG	2.2
2	H	393	PHE	2.2
2	H	64	GLU	2.2
1	C	36	GLY	2.2
2	D	376	ARG	2.2
2	H	151	GLU	2.1
2	B	21	THR	2.1
2	B	218	LYS	2.1
1	E	36	GLY	2.1
2	B	366	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	300	ARG	2.1
2	H	118	LEU	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^{th} 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	HTG	F	406	5/19	0.76	0.23	2.55	39,39,40,42	0
3	ZMP	A	99	36/37	0.86	0.17	1.37	24,27,33,34	0
4	HTG	D	406	5/19	0.84	0.18	1.37	23,24,24,25	0
3	ZMP	E	99	36/37	0.90	0.15	1.21	20,25,31,32	0
3	ZMP	C	99	36/37	0.91	0.15	0.73	25,28,32,33	0
3	ZMP	G	99	36/37	0.90	0.16	0.36	29,31,35,36	0
4	HTG	A	101	6/19	0.82	0.17	0.36	33,33,33,33	0
5	HEM	B	405	43/43	0.97	0.12	0.16	13,14,15,18	0
5	HEM	F	405	43/43	0.97	0.12	0.12	13,15,17,19	0
4	HTG	H	406	7/19	0.93	0.16	-0.03	41,42,43,43	0
4	HTG	E	100	16/19	0.91	0.14	-0.08	30,31,32,32	0
5	HEM	H	405	43/43	0.96	0.12	-0.12	15,16,18,19	0
5	HEM	D	405	43/43	0.97	0.11	-0.29	12,13,16,16	0
4	HTG	C	100	15/19	0.92	0.14	-0.45	38,39,40,40	0
4	HTG	A	100	14/19	0.92	0.11	-1.06	28,29,29,29	0
4	HTG	G	100	15/19	0.92	0.09	-1.43	31,33,33,34	0
6	CL	F	407	1/1	0.80	0.18	-	53,53,53,53	0
6	CL	B	406	1/1	0.61	0.19	-	53,53,53,53	0

6.5 Other polymers (i)

There are no such residues in this entry.